

ESRF Experiment Division Tuesday Events 15/09/2009



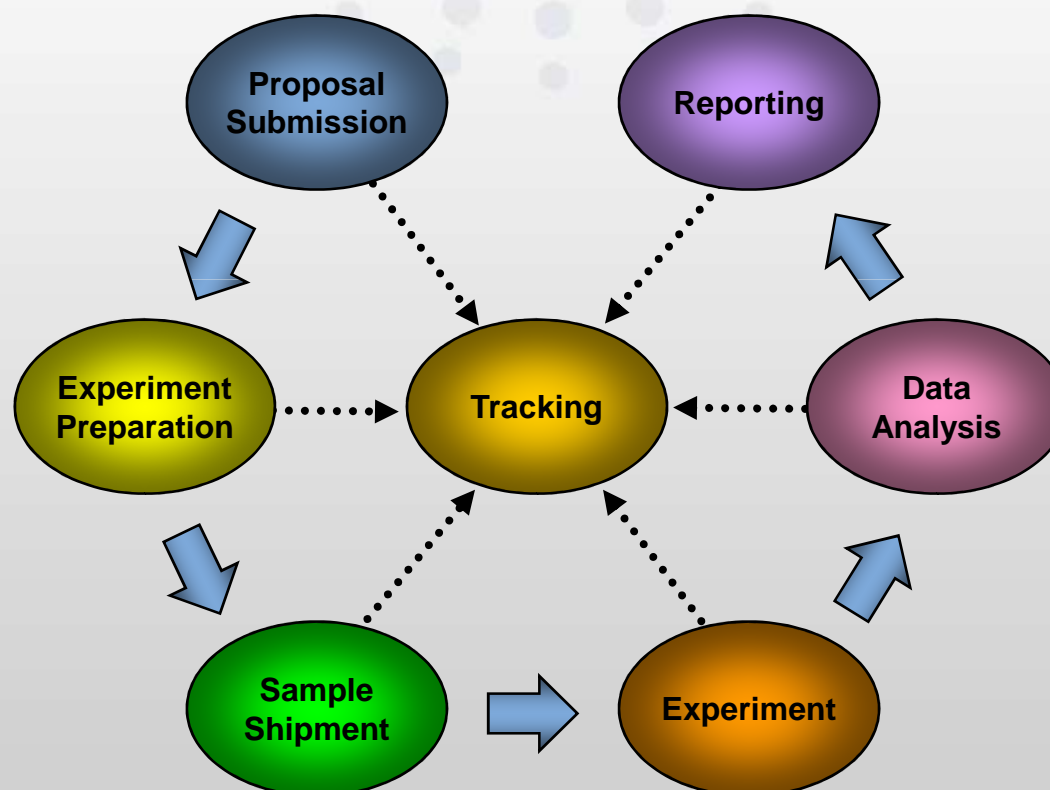
**From your sample to your data analysis: how to
track every step of your experiment in a database.
An example with ISPyB for MX experiments**

Patrice Brechereau ESRF/CS/MIS

Contents

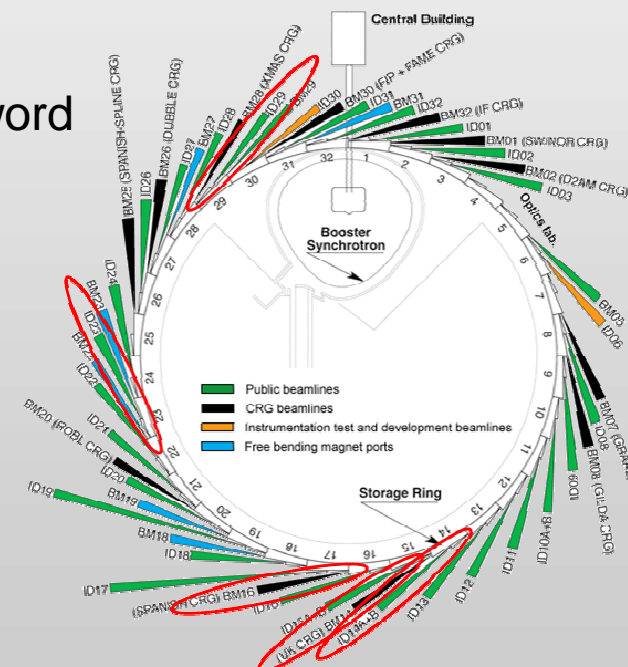
- Tracking, experiments, samples, data analysis...
- What is ISPyB?
- Features
- Architecture
- What's next?

From your sample to your data analysis: how to track every step of your experiment in a database...



What is ISPyB?

- ISPyB: Information **S**ystem for **P**rotein Crystallograph**Y** **B**eamlines
 - Laboratory Information Management System (LIMS) for protein crystallography experiments on synchrotron beamlines
 - Web based interface
- Access
 - <http://ispyb.esrf.fr>
 - To log-in: ESRF experiment number and password
- Where is it used at the ESRF?
 - ID14-1, ID14-2, ID14-4
 - ID14-3 soon (BioSAXS)
 - ID23-1, ID23-2, ID29
 - BM14, BM16



Proposals and Users

- Type of Proposals:
 - IX: Industrial Users who come to the ESRF
 - FX: Industrial Users who don't come to the ESRF (MXPress Service)
 - MX: Academic Users (mainly BAG / Block Allocation Group)
- ISPyB Users:
 - End user (users on site or remote, ESRF local contact)
 - Local Contacts (dewar tracking)
 - Fx Managers (managing Industrials)
 - Bloms (managing beamlines)
 - Stores (dewar tracking)

History

- 2001-2005: Pxweb
 - Python/Zope, MySql
 - JSBG Project (ESRF/EMBL)
 - Experiment logging for MXPress users (FX users)
- 2005-now: ISPyB
 - Java/Struts/Jboss, Mysql
 - ESRF/Spine/Bioxhit and BM14/MRC/eHTPX collaboration
 - Pxweb features + new features + Dewar Tracking
 - 2009: Collaboration with Diamond (code sharing)



diamond

EMBL



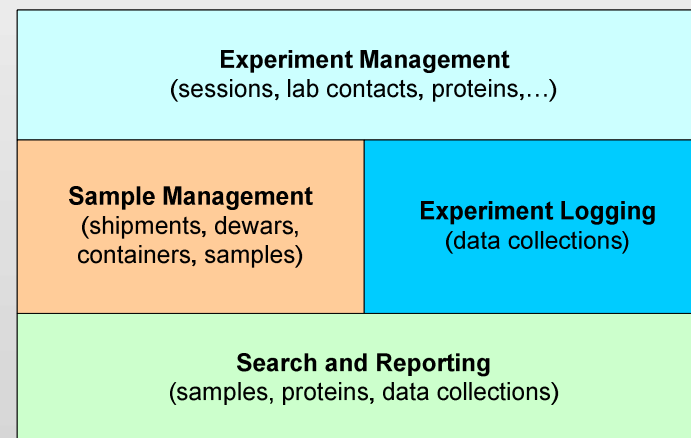
BIOXHIT

ISPyB Project Management

- Management Structure
 - Steering Committee
 - Executive Committee
 - Scientific and User Committee
 - Project Manager
 - Developers
- Meetings
 - ESRF / DLS once a month (Marratech)
 - Synchrotrons: every 6 months / 1 year (last was April 2009)
- Source Code
 - Shared on SourceForge / SVN
 - Bug & New Feature tracking
 - Site specific statements : `is_ESRF()`, `is_DLS()`

ISPyB Features & Modules

- Experiment Management
- Sample Management
- Experiment Recording
- Search and Reporting



Experiment Management

- Items:
 - Proposals
 - Sessions (date, beamline, local contact)
 - Lab Contacts (email, address,..)
 - Proteins (approved sample sheets)
- Features:
 - Data retrieved from the User Portal (SMIS)
 - Edit Lab Contact Card

Experiment Management (sessions, lab contacts, proteins,...)	
Sample Management (shipments, dewars, containers, samples)	Experiment Logging (data collections)
Search and Reporting (samples, proteins, data collections)	

Lab Contacts

Search

New/Edit LabContact

Scientist name

Scientist firstname

Select

Select the scientist contact

Scientist name	Scientist first name	Lab name	Action
TURKENBURG	J.P.	York Structural Biology Laboratory	Select
LEONARD	Gordon	E.S.R.F.	Select
MONACO	Stéphanie	E.S.R.F.	Select
TERRADOT-PIOT	Laurent	E.S.R.F.	Select
THIBAUT	Xavier	E.S.R.F.	Select
SPRUCE	Darren	E.S.R.F.	Select
GUIJARRO	Matias	E.S.R.F.	Select
PIPELINE	Data	E.S.R.F.	Select
CHA	Sun-shin	Pohang Accelerator Laboratory	Select
KIM	In-kwon	Department of Chemistry	Select
KIM	Min-Kyu	Laboratory of Biophysics	Select
AN	Young jun	Korea Ocean Research & Development Institute	Select
SEO	Koung hye	Department of Chemistry	Select
LEE	Kon ho	Gyeongsang National University	Select
KOSKI	Kristian	Department of Biochemistry	Select
HAAPALAINEN	Antti	Department of Biochemistry	Select
BUJACZ	Grzegorz	Institute of Bioorganic Chemistry	Select

Edit

New/Edit LabContact

Lab-contact card

Card name

Contact person info

Family name

First name

Telephone

Fax

Email

Laboratory info

Lab name

Lab address (*)

(*) address must fit in the text box without scrolling

Default info

Courier company for return (if ESRF sends a dewar back)

Courier account

Billing reference

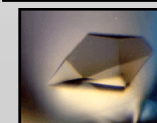
Average Customs value of a dewar (Euro)

Average Transport value of a dewar (Euro)

Sample Management

- Items:
 - Shipments (set of dewars)
 - Dewars (barcode, courier tracking number)
 - Containers (barcode)
 - Samples (barcode, protein acronym, crystal form,...)
- Features:
 - Online shipment description
 - Shipment description upload (Excel file)
 - Dewar Tracking

Experiment Management (sessions, lab contacts, proteins,...)	
Sample Management (shipments, dewars, containers, samples)	Experiment Logging (data collections)
Search and Reporting (samples, proteins, data collections)	



Creating Shipments

Shipment Creation

New/Edit Shipment

Details

Creation date: 2009-09-10

Shipment label: MyShipment

Number of dewars: 2

Number of other components (i.e. toolbox, laser...): 1

01-12-2009 ID14.4

Beamline / Experiment:

Comments: Thank!

Shipment status: opened

Lab-contacts

Lab-Contact for sending: MONACO-E.S.R.F.

Creation/Editing of a Lab-Contact card

Return address is identical as sending address (Y/N): ☒

If No, Lab-Contact for Return: MONACO-E.S.R.F.

Save

Shipment Description (Excel)

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1		Template version	5																
2		Puck		Puck1															
3		Dewar		Dewar1															
4		Proposal Id / Shipping Id	1084	302154															
5																			
6	Sample position	Protein Acronym - SpaceGroup	Space Group	Sample Name	Pin Barcode	Pre-observed Resolution	Header Resolution	Collision Range	Experiment Type	Anomalous Scatterer	a	b	c	alpha	beta	gamma	Loop Type	Holder Length	Comments
7	1	A-TM - P21		S1000	CA00AB2093				OSC		99.94	54.99	27.53	90.00	99.61	90.00	Nylon	22	
8	2	ABCDEF - P2221		S1001	HA00AA5311				OSC		26.60	41.61	54.05	83.29	84.26	74.36	Nylon	22	
9	3	3 - P6122		S1002	CA00AA2964				OSC		55.01	55.12	60.17	89.54	14.58	87.95	Nylon	22	
10	4								OSC								Nylon	22	
11	5	3 - I2121							OSC								Nylon	22	
12	6	3 - C2							OSC								Nylon	22	
13	7	3 - P6122							OSC								Nylon	22	
14	8	3 - F4132							OSC								Nylon	22	
15	9	3 - P21212							OSC								Nylon	22	
16	10	A-TM - P21							OSC								Nylon	22	
17		A-TM - P23							OSC								Nylon	22	

Dewar Labels (sending, return)

TO: ESRF Magasin
6 rue Jules Horowitz
38042 Grenoble
FRANCE
Tel: +33 (0)4 76 88 2733
Fax: +33 (0)4 76 88 2347

Frozen samples in Dry-Shipper for experiments at ESRF

Not restricted, As per IATA special provision A152

FRAGILE

THIS WAY UP

HANDLE WITH CARE DO NOT DROP

Parcel label: Dewar1

Shipment name: PBU100

Number of parcels: 1

Proposal number: PX399

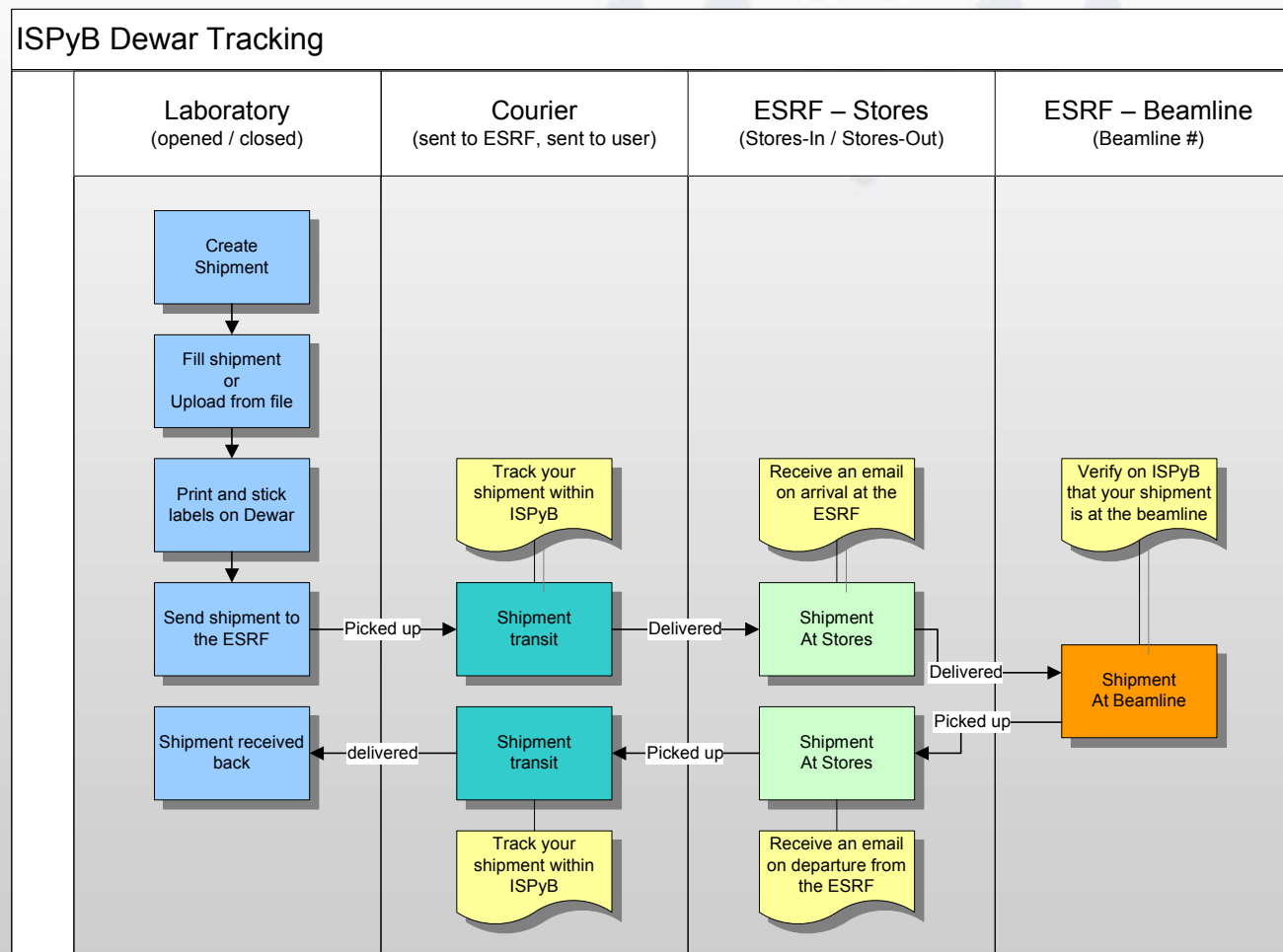
Beamline: ID29

Experiment date: 01-12-2009

Local contact: BRENCHEREAU P

FROM: (Lab-contact sending)
BRENCHEREAU Patrice
ESRF
Computing Services - MIS Group
E.S.R.F.
BP 220 - 8 rue Jules Horowitz
F-38043 Grenoble Cedex
Tel: +33 (0)476 88 2921 Fax:

Dewar Tracking



Dewar1 history view

Label	Dewar1
Barcode	ESRF0302349
Average customs values (Euro)	4000
Average transport values (Euro)	4000

Outbound courier

Outbound tracking number

Date	Status	Location
07-04-2009 10:54	ready to go	
17-04-2009 10:09	at ESRF	STORES-IN
17-04-2009 14:08	at ESRF	ID14
23-04-2009 11:26	at ESRF	STORES-OUT
23-04-2009 14:32	at ESRF	ID14
16-05-2009 21:42	ready to go	
18-05-2009 09:45	at ESRF	STORES-OUT
18-05-2009 11:46	sent to User	

Return courier

Return tracking number

Fedex
796614000970

FedEx

Experiment Recording

Experiment Management (sessions, lab contacts, proteins,...)	
Sample Management (shipments, dewars, containers, samples)	Experiment Logging (data collections)
Search and Reporting (samples, proteins, data collections)	

- Items:
 - Session info (date, beamline name, operator,...)
 - Experiment parameters (wavelength, energy, detector distance,...)
 - Beamline parameters (name, beam transmission, beam size,...)
 - Crystal snapshots
 - Images (thumbnails, link to real images)
 - Data Analysis / EDNA results (characterisation & strategy, mosflm.log, pointless.log,...)

Data Collections

Data Collections of a Session

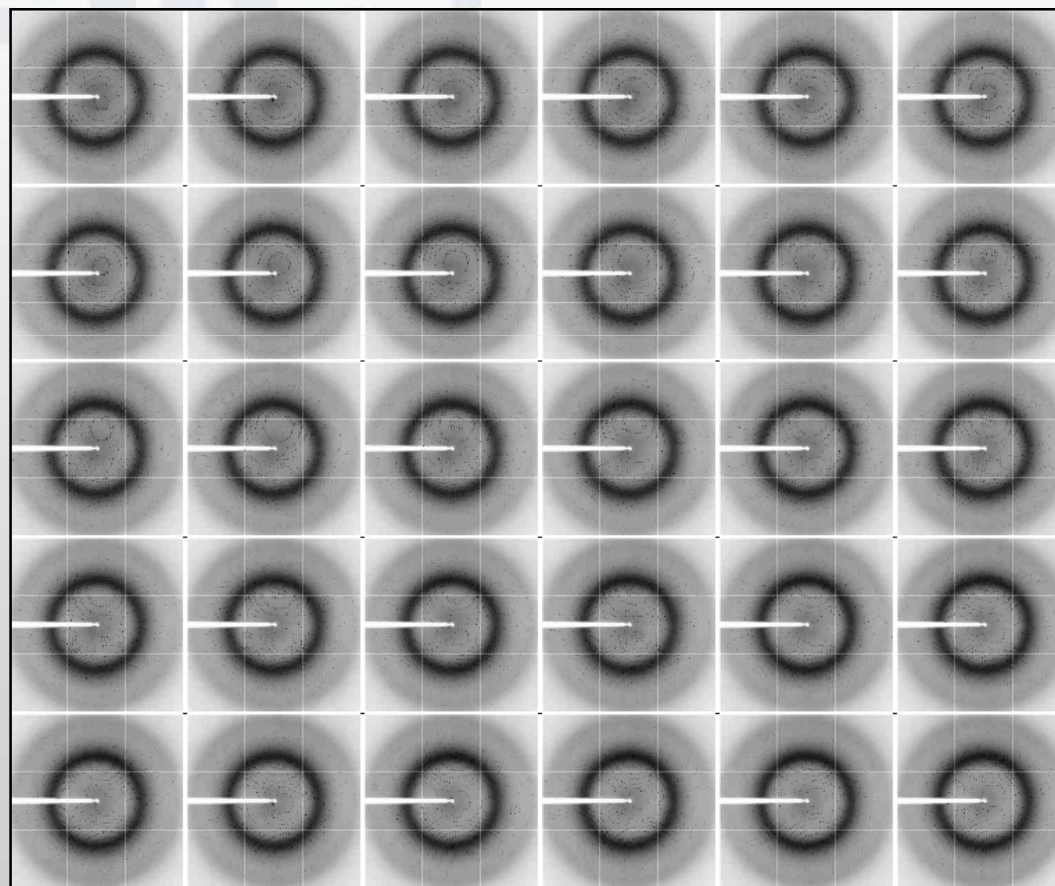
- This collection has a crystal snapshot.
- collection successful
- DNA indexing failed.
- No samples for the data collection.

Data Collections

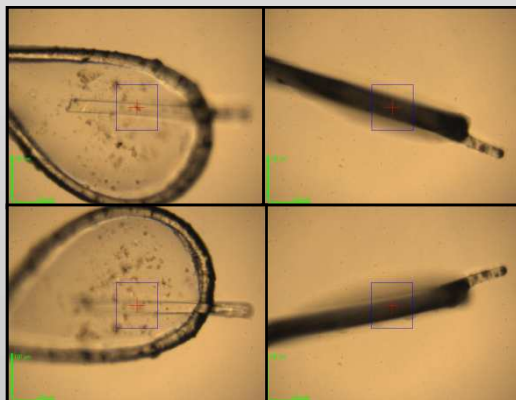
Parameters & Results

Experiment parameters	Beamline parameters	DNA results
Img directory /data/visitor/mx415/id14eh4/20090909/SAD		
Img prefix stand-fae		
Run no 3		
Start Time 09-09-2009 11:27:53		
End Time 09-09-2009 11:39:01		
Type of experiment		
Wavelength 0.9795 Å		
Energy 12.658 keV		
Phi start 167.0°		
Oscillation range 0.75°		
Overlap 0.0°		
Exposure Time 0.5 s		
Number of passes 1		
Detector Distance 287.9 mm		
Resolution at edge 1.99 Å		
Resolution at corner 1.52 Å		
Xbeam 157.72 mm		
Ybeam 156.91 mm		
Detector 2theta 0.0		
Kappa N/A		
Phi N/A		
Experiment comment DNA data collection		

Image thumbnails (image wall)



Crystal Snapshots



Search and Reporting

- Search
 - Data Collection (protein, sample, experiment date,...)
 - Proteins
 - Samples
- Reports
 - Pdf, Word, Csv

Experiment Management (sessions, lab contacts, proteins,...)	
Sample Management (shipments, dewars, containers, samples)	Experiment Logging (data collections)
Search and Reporting (samples, proteins, data collections)	





Search

Protein or Sample

Search Protein

Acronym



Protein	Space Group	Sample name	Smp. code	Shipment	Device	Container	Loc. in cont.	Cell a	Cell b	Cell c	Cell alpha	Cell beta	Cell gamma	Crystal comments	Already observed	Minimal resol.	Sample comments	Edit sample	Sample status	Data Collections
FAE	P212121	Se01	HA00A18881	Test Xtals 0607	MX Group	CA380A	1	65.4	108.8	113.9	90.0	90.0	90.0		0	0		Edit Delete		
FAE	P212121	Se02	HA00A18880	Test Xtals 0607	MX Group	CA380A	2	65.4	108.8	113.9	90.0	90.0	90.0		0	0		Edit Delete	COL_2007-11-12	
FAE	P212121	Se03	HA00A18889	Test Xtals 0607	MX Group	CA380A	3	65.4	108.8	113.9	90.0	90.0	90.0		0	0		Edit Delete	TEST_2007-07-04	
FAE	P212121	Se04	HA00A18888	Test Xtals 0607	MX Group	CA380A		65.4	108.8	113.9	90.0	90.0	90.0		0	0		Edit Delete	TEST_2008-02-18	
FAE	P212121	Se05	HA00A18887	Test Xtals 0607	MX Group	CA380A		65.4	108.8	113.9	90.0	90.0	90.0		0	0		Edit Delete		
FAE	P212121	Se06	HA00A18886	Test Xtals 0607	MX Group	CA380A		65.4	108.8	113.9	90.0	90.0	90.0		0	0		Edit Delete		
FAE	P212121	Se07	HA00A18882	Test Xtals 0607	MX Group	CA380A		65.4	108.8	113.9	90.0	90.0	90.0		0	0		Edit Delete		
FAE	P212121	Se08	HA00A18885	Test Xtals 0607	MX Group	CA380A		65.4	108.8	113.9	90.0	90.0	90.0		0	0		Edit Delete		
FAE	P212121	Se09	HA00A18854	Test Xtals 0607	MX Group	CA380A		65.4	108.8	113.9	90.0	90.0	90.0		0	0		Edit Delete		
FAE	P212121	Se10	HA00A18853	Test Xtals 0607	MX Group	CA380A		65.4	108.8	113.9	90.0	90.0	90.0		0	0		Edit Delete		
FAE	P212121	Se11	HA00A19072	Test Xtals 0607	MX Group	CA391A		65.4	108.0	113.9	90.0	90.0	90.0		0	0		Edit Delete	COL_2007-09-21	



Data Collection



Search datacollection

Sample name:

Protein acronym:

Beamline:

Experiment date between DD-MM-YYYY:  

and DD-MM-YYYY:  



Min number of images:

Max number of images:

Max Data Collections retrieved:

You may use the * character to do a search with an incomplete Name.



 Image Prefix	Run No	Protein Acronym	 Start Time	# images	Wavelength	Transm.	Distance	Ex. Time	Phi start	Phi range	Xbeam	Ybeam	Detector Resolution	Status	Sample Ranking	Comment
		<div>FAE</div>													<div>Rank</div>	
FAE-X35	3	FAE	08-07-2009 13:26:14	209	0,976	100	211,7	0,07	67	0,45	159,19	165,34	1,62	<div><div></div><div></div><div></div><div></div></div>	<div><div></div></div>	DNA data collection
ref-FAE-X35	2	FAE	08-07-2009 13:24:31	2	0,976	100	226,01	1	0	1	159,18	165,36	1,7	<div><div></div><div></div><div></div><div></div></div>	<div><div>✓</div></div>	Collecting 2 reference images
ref-FAE-X35	1	FAE	08-07-2009 13:00:55	2	0,976	100	226,01	1	0	1	159,18	165,36	1,7	<div><div></div><div></div><div></div><div></div></div>	<div><div>✓</div></div>	Collecting 2 reference images
test	2	FAE	19-05-2009 16:49:43	1	0,873	100	504,72	1	0	1	112,55	112,14	4	<div><div></div><div></div><div></div><div></div></div>	<div><div></div></div>	
test	1	FAE	19-05-2009 16:49:03	1	0,873	100	504,72	1	0	1	112,55	112,14	4	<div><div></div><div></div><div></div><div></div></div>	<div><div></div></div>	
FAE-X1	1	FAE	19-05-2009 11:31:41	1	0,873	100	635,22	1	0	1	112,42	112,11	5	<div><div></div><div></div><div></div><div></div></div>	<div><div></div></div>	
FAE-XFAE11	1	FAE	07-04-2009 19:47:47	1	0,933	100	299,8	1	0	1	94,6	95,45	3,13	<div><div></div><div></div><div></div><div></div></div>	<div><div></div></div>	
FAE-XFAE21	2	FAE	01-04-2009 15:03:22	103	0,933	100	178,61	0,07	151	0,7	94,47	95,38	1,97	<div><div></div><div></div><div></div><div></div></div>	<div><div></div></div>	DNA data collection
postref-FAE-XFAE21	2	FAE	01-04-2009 15:02:39	3	0,933	100	178,61	0,07	241	0,7	94,47	95,38	1,97	<div><div></div><div></div><div></div><div></div></div>	<div><div></div></div>	
ref-FAE-XFAE21	1	FAE	01-04-2009 15:00:25	2	0,933	100	181,86	1	0	1	94,47	95,39	2	<div><div></div><div></div><div></div><div></div></div>	<div><div>✓</div></div>	Collecting 2 reference images
ref-FAE-XFAE21	1	FAE	01-04-2009 14:58:42	2	0,933	2,1	181,95	1	0	1	94,47	95,39	2	<div><div></div><div></div><div></div><div></div></div>	<div><div></div></div>	Collecting 2 reference images

Reporting

Pdf

Word

Pdf

Data Collections for Proposal: mx415 on Beamline: ID23-1 --- Session start date: 06-07-2009

Session comments:
Session created by the BCM

Image prefix	Run no.	# Images	Wavelength (nm)	Distance (mm)	Exp. Time (sec)	Phi start (deg)	Phi range (deg)	Xbeam (mm)	Ybeam (mm)	Detector (mm)	Comments
ins	2	14	0.976	197.60	0.34	115.95	0.35	189.19	185.25	1.84	
ins	1	87	0.976	197.61	0.10	99.00	0.35	189.19	185.25	1.84	
ref-ins	2	2	0.976	190.44	1.00	0.00	1.00	189.20	186.31	1.60	Collecting 2 reference images
ref-ins	1	2	0.976	226.00	1.00	0.00	1.00	189.18	186.36	1.70	Collecting 2 reference images
FAE-X35	4	21	0.976	226.35	0.65	112.95	0.80	189.18	186.36	1.70	
FAE-X35	3	31	0.976								
FAE-X35	2	22	0.976								
FAE-X35	1	80	0.976								
ref-FAE-X35-3	1	2	0.976								
ref-FAE-X35	3	2	0.976								
FAE-X35-2	6	46	0.976								
FAE-X35-2	5	42	0.976								
FAE-X35-2	4	51	0.976								
FAE-X35-2	3	15	0.976								
FAE-X35-2	2	13	0.976								
ref-FAE-X35-2	1	2	0.976								
FAE-X35	3	209	0.976								
ref-FAE-X35	2	2	0.976								
ref-FAE-X35	1	2	0.976								
mx415	2	348	0.976								
postref-mx415	2	2	0.976								
ref-mx415	1	2	0.976								
FAE-X34	3	1	0.976								
FAE-X34	2	1	0.976								
FAE-X34	1	1	0.976								
beamstop	2	1	0.976								
beamstop	1	1	0.976								

Coverings for Proposal: mx415 on Beamline: ID23-1 --- Session start date: 06-07-2009

Image prefix	Run no.	# Images	Wavelength (nm)	Distance (mm)	Exp. Time (sec)	Phi start (deg)	Phi range (deg)	Beam Size X (mm)	Beam Size Y (mm)	Detector (mm)	Comments
ref-FAE-X35-3	1	2	0.976	226.03	1.00	0.00	1.00	0.00	0.00	1.70	Collecting 2 reference images

3/14/2009 14:15:15

img SpaceGroup: P222
1/2: 06.18 109.61 114.85 90.00 90.00 90.00 0.40 1.82 5.90

Indexing successful

Phi Start: 18.0 Phi End: 129.6 Rotation: 0.2 Exp. Time: 0.4 Data Res: 1.83 Tot. Exp. Time: 210.8 Tot. No. img: 525 Program: BESS 3.1.0c

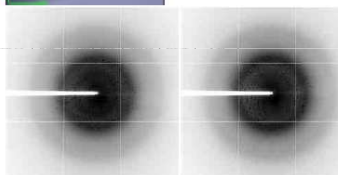
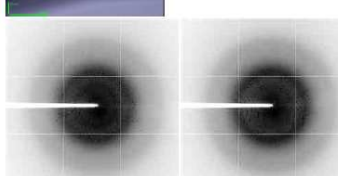

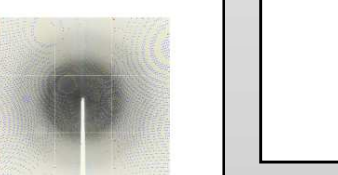





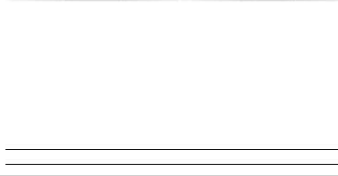
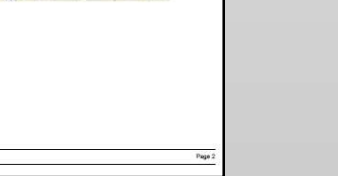
Image prefix	Run no.	# Images	Wavelength (nm)	Distance (mm)	Exp. Time (sec)	Phi start (deg)	Phi range (deg)	Beam Size X (mm)	Beam Size Y (mm)	Detector (mm)	Comments
ref-FAE-X35	3	2	0.976	226.05	1.00	0.00	1.00	0.00	0.00	1.70	Collecting 2 reference images

3/14/2009 14:15:22

img SpaceGroup: P222
1/2: 06.15 109.55 114.84 90.00 90.00 90.00 0.38 1.58 5.90

Indexing successful

Phi Start: 18.0 Phi End: 129.6 Rotation: 0.2 Exp. Time: 0.2 Data Res: 1.82 Tot. Exp. Time: 111.3 Tot. No. img: 525 Program: BESS 3.1.0c

Session logs for mx415 on ID23-1 Date: 06-07-2009

Image prefix	Run #	# Images	Wavelength (nm)	Distance (mm)	Exp. Time (sec)	Phi Start (deg)	Phi Range (deg)	Beam Size X (mm)	Beam Size Y (mm)	Resolution (nm)	Collecting 2 reference images
ref-FAE-X35-3	1	2	0.976	226.03	1.00	0.00	1.00	0.00	0.00	1.70	

3/6/2009 14:16:15

Indexing successful

img	Space Group	a	b	c	alpha	beta	gamma	Mosaicity	Obs. Res.
1-2	P222	66.18	109.61	114.85	90.00	90.00	90.00	0.40	1.82

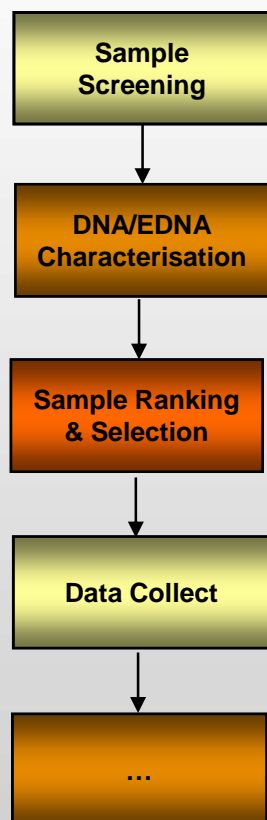
Phi Start	Phi End	Rotation	Exp. Time	Strategy Res.	Tot. Exp. Time	Tot. No. img	Program
18.0							

	A	B	C	D	E	F	G	H	I	J	K	L
1	Image prefix	Beamline	Run no	Start Time	Sample No	Protein Ac	# images	Wavelength	Distance (mm)	Exp. Time (sec)	Phi start (deg)	Phi range (deg)
2	ins	ID23 1	2	8/7/2009 17:15			14	0.976	197.6	0.34	115.95	0.3
3	ins	ID23 1	1	8/7/2009 17:14			57	0.976	197.61	0.1	96	0.35
4	ref-ins	ID23 1	2	8/7/2009 17:05			2	0.976	190.44	1	0	1
5	ref-ins	ID23 1	1	8/7/2009 16:54			2	0.976	226	1	0	1
6	FAE-X35	ID23 1	4	8/7/2009 14:42			21	0.976	226.35	0.65	112.95	0.5
7	FAE-X35	ID23 1	3	8/7/2009 14:41			31	0.976	226.35	0.4	92.8	0.65
8	FAE-X35	ID23 1	2	8/7/2009 14:40			22	0.976	226.35	0.31	63	0.9
9	FAE-X35	ID23 1	1	8/7/2009 14:38			80	0.976	226.35	0.1	33	0.5
10	ref-FAE-X35-3	ID23 1	1	8/7/2009 14:16			2	0.976	226	1	0	1
11	ref-FAE-X35	ID23 1	3	8/7/2009 14:12			2	0.976	225.95	1	0	1
12	FAE-X35-2	ID23 1	6	8/7/2009 14:02			46	0.976	251.3	0.55	103.75	0.45
13	FAE-X35-2	ID23 1	5	8/7/2009 14:00			42	0.976	251.3	0.37	74.35	0.7
14	FAE-X35-2	ID23 1	4	8/7/2009 13:58			51	0.976	251.3	0.13	53.95	0.4
15	FAE-X35-2	ID23 1	3	8/7/2009 13:58			15	0.976	251.3	0.18	44.2	0.65
16	FAE-X35-2	ID23 1	2	8/7/2009 13:57			13	0.976	251.37	0.1	39	0.4
17	ref-FAE-X35-2	ID23 1	1	8/7/2009 13:39			2	0.976	226.04	1	0	1
18	FAE-X35	ID23 1	3	8/7/2009 13:26 X35	FAE		209	0.976	211.7	0.07	67	0.45
19	ref-FAE-X35	ID23 1	2	8/7/2009 13:24 X35	FAE		2	0.976	226.01	1	0	1
20	ref-FAE-X35	ID23 1	1	8/7/2009 13:00 X35	FAE		2	0.976	226.01	1	0	1
21	mx415	ID23 1	2	8/7/2009 12:05			348	0.976	225.66	0.05	131	0.55
22	postref-mx415	ID23 1	2	8/7/2009 12:04			3	0.976	225.62	0.05	221	0.55
23	ref-mx415	ID23 1	1	8/7/2009 11:56			2	0.976	242.39	0.5	0	1
24	FAE-X34	ID23 1	3	8/7/2009 11:50			1	0.976	276.56	1	0	5
25	FAE-X34	ID23 1	2	8/7/2009 11:43			1	0.976	276.56	1	0	0.1
26	FAE-X34	ID23 1	1	8/7/2009 11:33			1	0.976	276.56	1	0	1
27	beamstop	ID23 1	2	8/7/2009 10:09			1	0.976	242.39	1	0	1
28	beamstop	ID23 1	1	8/7/2009 10:08			1	0.976	242.39	1	0	1
29												
30												

Excel / Csv

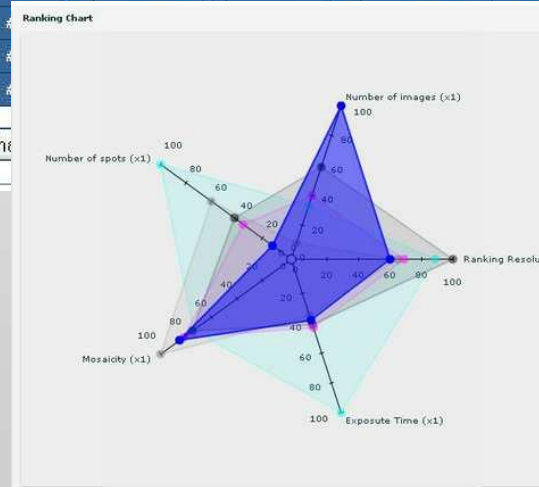
Sample Ranking

Ranked Samples



Sample Ranking (Rank - Value)

Select Sample	Image Prefix	Run No	Start time	Space Group	UC a	UC b	UC c	Ranking resol. Å	Exposure time s	Mosaicity	Number of spots	Number of images	Total
<input checked="" type="checkbox"/>	ref-t2-35b1-2	1	10:15:50	C2221	70	206	107	#2 2.24	#1 223.0	#3 0.54	#1 2606	#8 107	#1 65 %
<input checked="" type="checkbox"/>	ref-p2_7_dna	1	15:31:14	P4	66	66	101	#1 1.99	#4 547.5	#2 0.53	#6 1107	#2 61	#2 70 %
<input checked="" type="checkbox"/>	ref-dna-HA00AQ0066	1	16:09:47	P222	65	126	230	#8 3.08	#9 604.0	#8 0.72	#13 510	#1 48	#3 58 %
<input checked="" type="checkbox"/>	ref-t2-35d6-1	4	11:25:50	P2	74	107	102	#10 3.34	#10 618.3	#1 0.48	#10 775	#5 80	#4 57 %
<input checked="" type="checkbox"/>	ref-mfe1f11b	1	20:16:36	P222	66	126	229	#5 2.85	#3 470.8	#2 0.53	#11 755	#7 99	#5 57 %
<input type="checkbox"/>	ref-t2-35d6-1	1	10:19:09	P2	74	107	102	#7 2.99	#6 585.1	#9 0.74	#7 1100	#3 70	#6 56 %
<input type="checkbox"/>	ref-mfe1f19b	1	20:34:00	P222	65	126	230	#3 2.81	#2 386.0	#5 0.62	#4 1259	#13 830	#7 52 %
<input type="checkbox"/>	ref-t2-35d6-1	2	10:38:23	P2	74	107	102	#9 3.12	#11 631.4	#10 0.82	#9 849	#4 74	#8 51 %
<input type="checkbox"/>	ref-t2-35d5	1	10:26:32	P2	74	107	102	#10 3.34	#13 647.5	#7 0.70	#5 1129	#6 98	#9 51 %
<input type="checkbox"/>	ref-mfe1f19b	2	20:35:55	P222	65	126	230	#4 2.84	#8 597.4	#5 0.62	#3 1558	#11 760	#10 50 %
<input type="checkbox"/>	ref-dna-HA00AC1704	1	16:06:19	P222	65	126	230						
<input type="checkbox"/>	ref-mfe1-rpmfe1f1-11	1	16:13:15	P222	66	126	229						
<input type="checkbox"/>	ref-t2-35d6-2	1	10:23:13	P2	75	107	102						

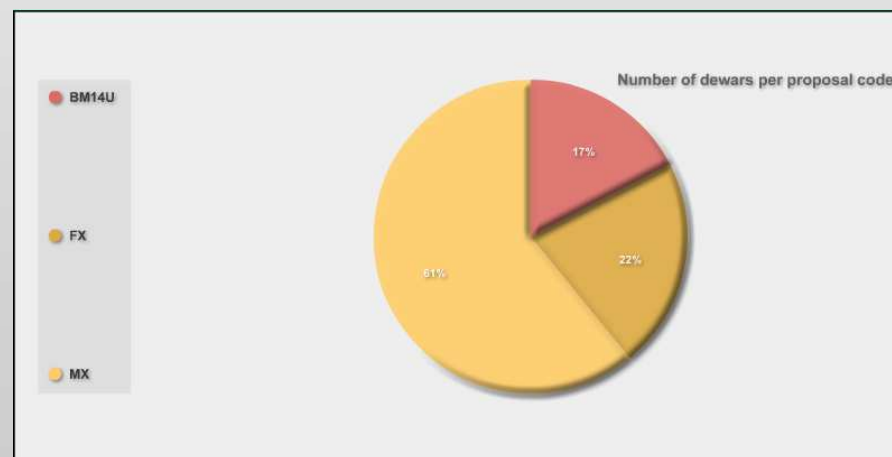
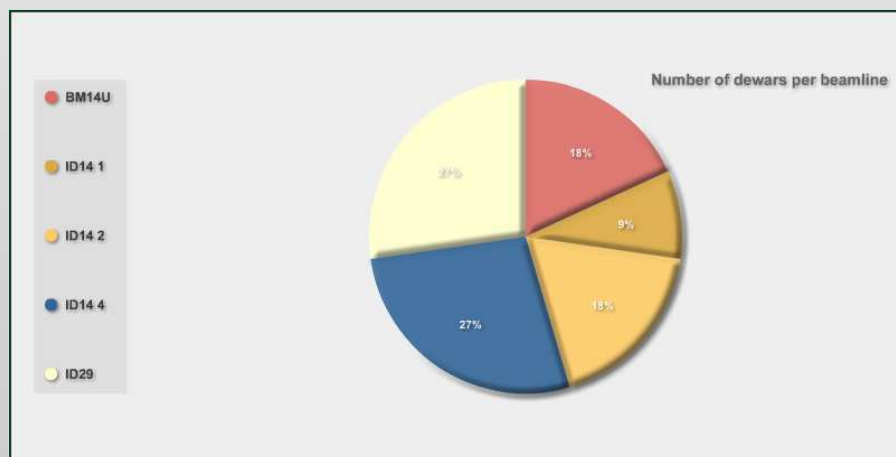
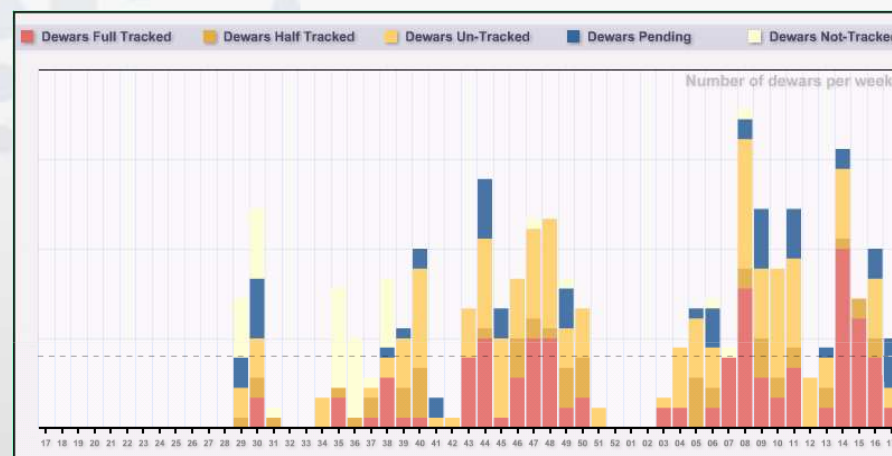
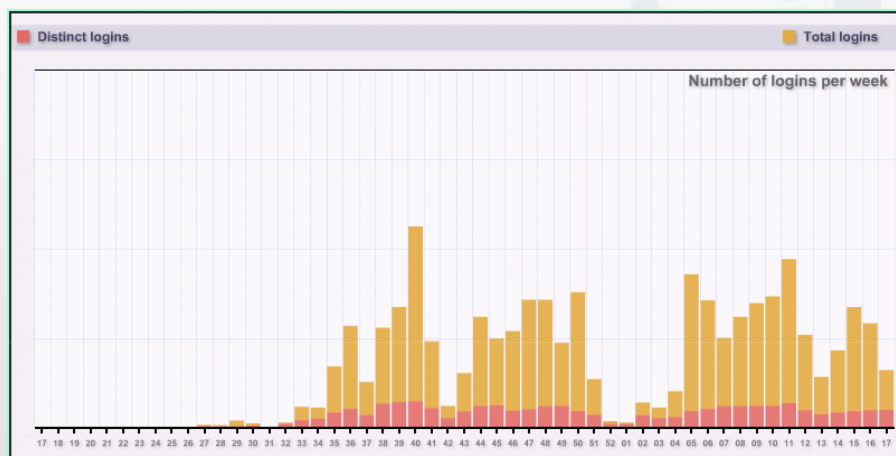


Sample List

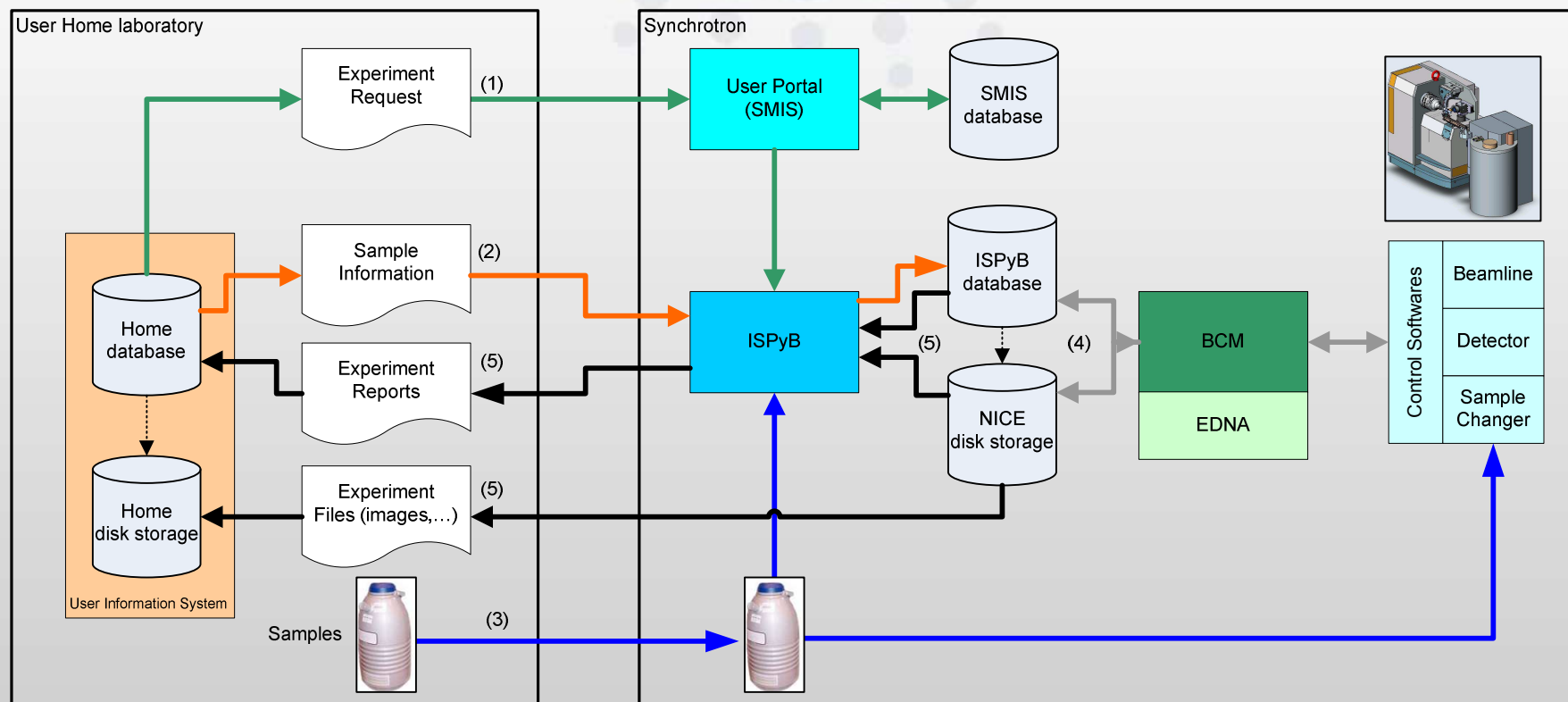
Colour	Select	Rank	Score	Image prefix	Sp	Re
<input checked="" type="checkbox"/>	1	79		ref-t2-35b1-2	C..	1
<input checked="" type="checkbox"/>	2	64		ref-p2_7_dna	P4	1
<input checked="" type="checkbox"/>	3	59		ref-mfe1f17	P..	1
<input checked="" type="checkbox"/>	4	54		ref-mfe1f16	P..	1
<input checked="" type="checkbox"/>	5	54		ref-mfe1-rpmf...	P..	1
<input type="checkbox"/>	6	53		ref-mfe1f16b	P..	3
<input type="checkbox"/>	7	52		ref-mfe1-rpmf...	P..	1
<input type="checkbox"/>	8	52		ref-mfe1-rpmf...	P..	1
<input type="checkbox"/>	9	52		ref-mfe1f11b	P..	1
<input type="checkbox"/>	10	51		ref-t2-35d6-1	P2	4
<input type="checkbox"/>	11	51		ref-mfe1-rpmf...	P..	1
<input type="checkbox"/>	12	50		ref-t2-35d6-1	P2	1
<input type="checkbox"/>	13	50		ref-dna-HA00A...	P..	1
<input type="checkbox"/>	14	50		ref-mfe1f11a	P..	2
<input type="checkbox"/>	15	49		ref-mfe1f19b	P..	1
<input type="checkbox"/>	16	47		ref-mfe1f19b	P..	2
<input type="checkbox"/>	17	47		ref-mfe1f16a	P..	1
<input type="checkbox"/>	18	47		ref-dna-HA00A...	P..	1
<input type="checkbox"/>	19	46		ref-t2-35d5	P2	1

Submit Cancel

Reporting for Managers Dashboard



Application Environment and Data Flow



ISPyB Data Model



ISPyB Technology

- Pure Web Interface
- Java
- Jboss Application Server (Ejb)
- Struts (MVC Web Application Framework)
- MySql / Oracle Database
- Communication with User Portal (SMIS) via Web Services
- Communication with BCM and EDNA
 - Through the Data Base
 - ...soon via Web Services



How does it help?

- Users
 - Prepare Experiment
 - Remote tracking by colleagues at home while the experiment is performed
 - Process experiment results back into the Home LIMS
 - Long term tracking of experiments (stored in the database)
- Communication between Users and ESRF Operations
 - Dewar description (beamline, local contact, user address)
 - Sample description (description, bar-code, location, known unit cell dimensions, space group, diffraction plans, comments)
 - Operator comments on data collections
- Safety (Dewar Tracking)

Next Steps...

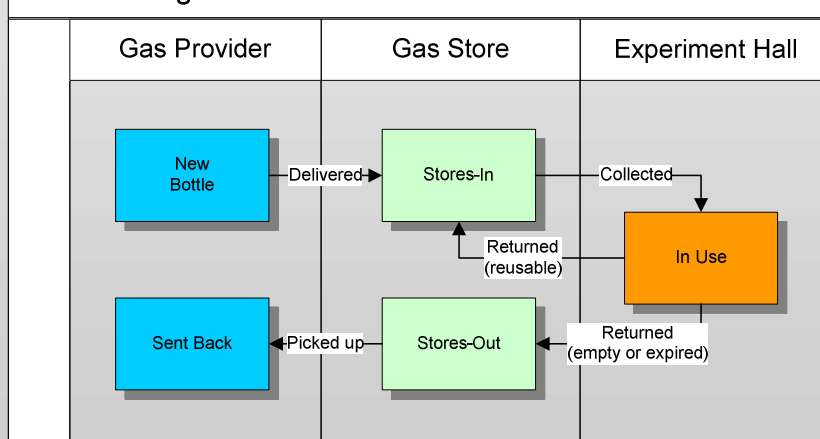
- ISPyB new features (new EDNA data, AutoProcessing,...)
- Object Tracking
- ISPyB for BioSAXS (ID14-3)
- ISPyB for other beamlines
- ISPyB for other MX facilities
- ISPyB and UPBL10/MASSIF

Gas Tracking

- Why Tracking bottles of gas?
 - Gas available at storage -> Users
 - Location of old bottles -> Safety, Finance
 - Location of 'dangerous' bottles -> Safety
- Uses Dewar Tracking architecture and technology



Gas Tracking Workflow





Welcome stores

Gas Tracking System

View bottles | Bottle charts

View bottles

Search

All

Stores-In

Stores-Out

In use

Sent back

Expired

Home

Logout

Contact

Copyright © 2009 ESRF

Search query

Select search values

Barcode:

Type:

Size:

Provider:

User:

Status:

Arrival between: and:

Expire between: and:

Sent back between: and:

Search Reset

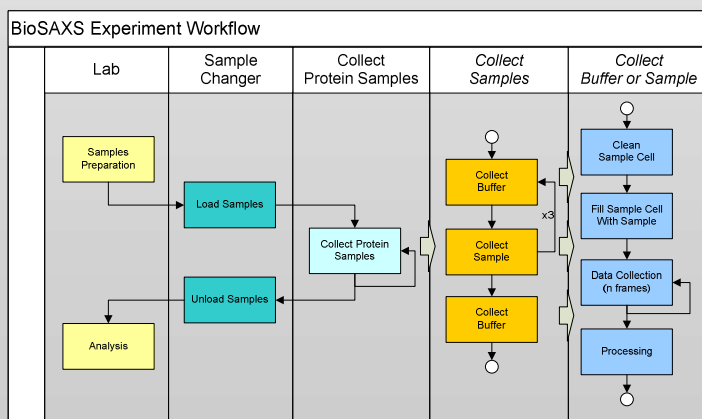
Search result: 4 bottles found

Barcode	Type	Size	Provider	User	Status	Arrival	Expiration	Exit	Actions
00000005	H2	B20	TEST	PATRICE	In use	31/08/2009	01/01/2010		x i
00000003	CO2	B10	TEST	...	Stores-In	31/08/2009	01/01/2010		x i
00000002	H2	B10	TEST	...	Stores-In	31/08/2009	01/01/2010		x i
00000001	CO2	B20	OTHER	...	Sent back	31/08/2009	01/01/2010	31/08/2009	x i

ISPyB For BioSAXS (ID14-3)

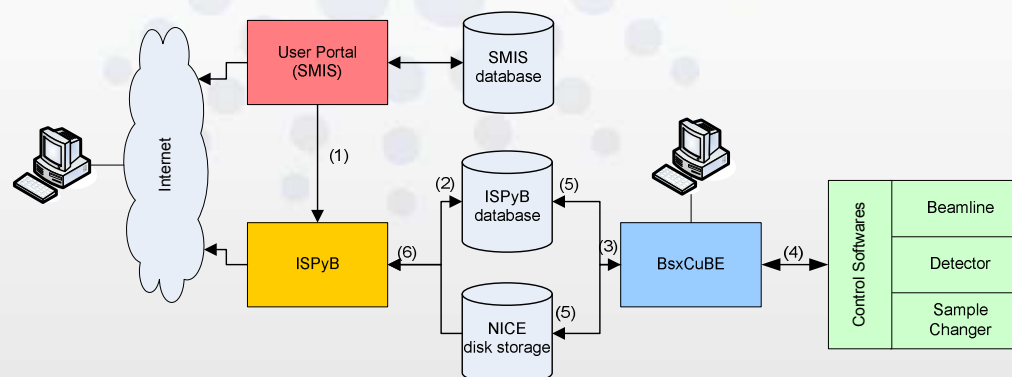


- BioSAXS needs
 - Sample Tracking
 - Experiment Management (sample preparation, ...)
 - Experiment Recording (images, data files, beamline parameters,...)
 - Search and statistics on past experiments
 - Web interface (remote access)
 - Link with MX experiments and SANS experiments...



ISPyB For BioSAXS (ID14-3)

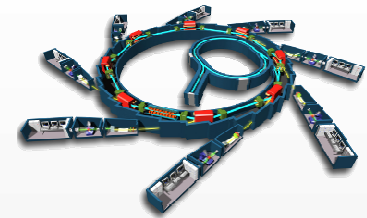
- Architecture



- Developments

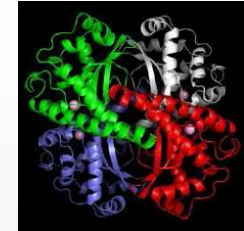
- Experiment Management: as it is in ISPyB
 - Sample Management: little customization (dewar/box, container/plate)
 - Experiment Management:
 - Data model extensions for BioSAXS data
 - GUI for BioSAXS data
 - Search and Report: customization for BioSAXS data
 - BCM/BsxCuBE evolutions
- An opportunity to see how we can use the ISPyB 'framework' and data model on other beamlines

ISPyB for Other Beamlines



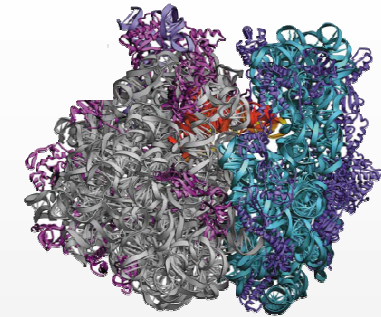
- Features
 - Sample Tracking
 - Experiment Logging
- Developments
 - Experiment Management: as it is in ISPyB (link with User Portal/SMIS)
 - Sample Management: beamline sample description (generic ?)
 - Experiment Recording
 - Experiment data model (one per experiment type ... or generic data model)
 - Gui to browse & view data collections
 - Search and Reports: depends on experiment data model
 - BCM (Beamline Control Management)
 - MX: MxCuBE
 - BioSAXS: BsxCuBE
 - ...

ISPyB Light for Other MX Facilities



- Facilities interested in using ISPyB
 - Max-Lab, Bessy, Soleil, APS,... (ISPyB meeting, April 2009)
- Features
 - Sample Management: as it is in ISPyB
 - Experiment Recording: as it is in ISPyB
 - Search and Report: as it is in ISPyB
 - Experiment Management: link with Proposal Submission System
 - Proposals, Sessions, Lab Contacts, Sample sheets,...
 - Current ISPyB: data filled in by User Portal / SMIS
 - ISPyB Light: API or Gui to fill in / manage this information

UPBL10 / MASSIF



- Many more samples...
 - Instead of a few samples, hundreds will be evaluated to select the best ones for data collection
 - An order of magnitude increase in samples and data
- ...and new Architecture / Workflow
 - Automated end stations for sample screening
 - End station for data collection
- Needs
 - As automation increased – more reliant on information from user (crystal mounting, size, composition,...)
 - Automated links with Home Lab Systems
 - Tracking by individual Samples
 - Sample Ranking (over hundreds of samples)
 - New data arrangement: not by session, by project ?
 - Sample Management: sorting facility associated with beamlines

Thanks to...

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ESRF
ESRF
ESRF
ESRF
ESRF
EMBL
ESRF

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ESRF
ESRF
ESRF

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ESRF
ESRF
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DLS
DLS

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ESRF
MRC/BM14
ESRF
ESRF
ESRF
ESRF

Oleg Konovalov

ESRF

... people I don't know but who have contributed to ISPyB
... people I forgot to mention (sorry)
... and all users for their constructive feedbacks

Questions...