

ISPYB: Information System for Protein CrystallographY Beamlines

LIMs for Macromolecular crystallography beamlines

What is ISPyB?

Access

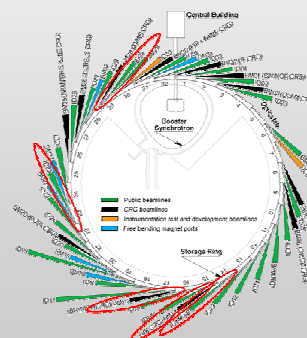
- <http://ispyb.esrf.fr>
- To log-in: ESRF experiment number and password

Where is it used ?

- ID14-1, ID14-2, ID14-4, ID23-1, ID23-2, ID29
- BM14, BM16
- Diamond

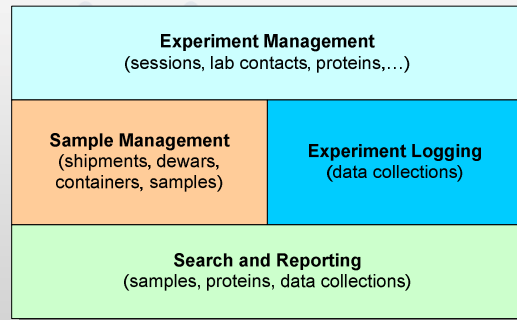
Coming soon at

- ID14-3 (BioSAXS)
- Hamburg (Petra III)

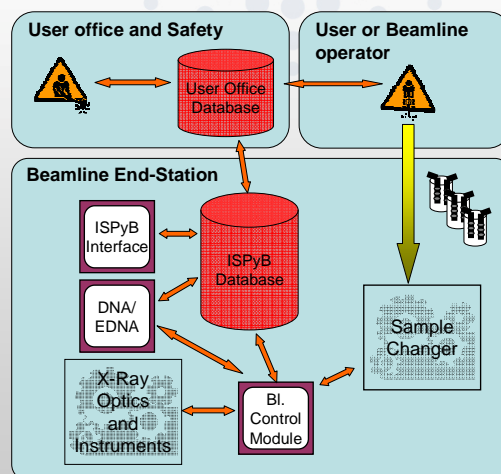


ISPyB Features & Modules

Experiment Management
Sample Management
Experiment Recording
Search and Reporting



The beamline



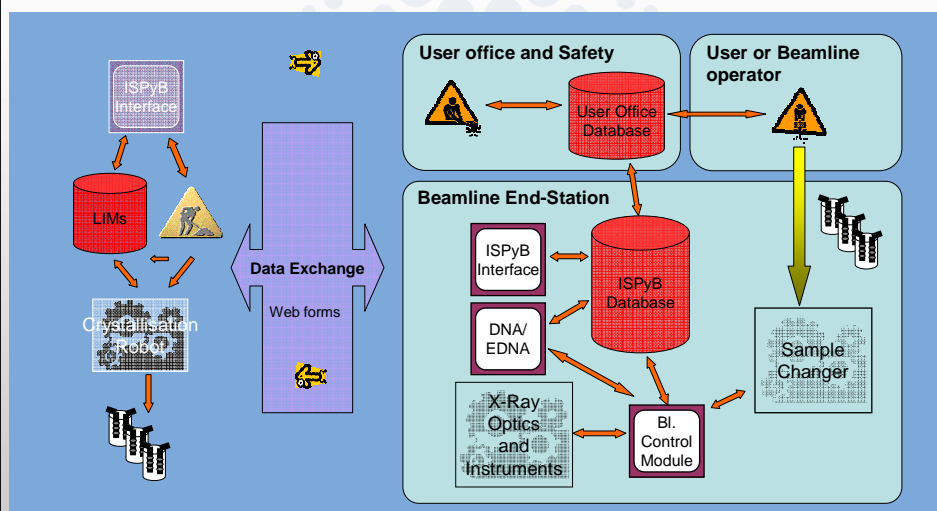
Most basic function - Experimental logging

The screenshot displays the ISPyB web interface for experimental logging. The browser address bar shows the URL: <http://ispyb.esrf.fr:8080/ispyb/user/viewDataCollection.do?reqCode=displayForSession&sessionId=26215>. The interface includes a sidebar with navigation links: Data collection, View last sessions, View all sessions, and Search data collections. The main content area shows a table of data collections with columns: Run ID, Program, Start Time, # images, Wavelength, Trans, Ex. #, #1, #2, Detector, Status, Sample, and Comments. A red circle highlights the first three rows of the table.

Run ID	Program	Start Time	# images	Wavelength	Trans	Ex. #	#1	#2	Detector	Status	Sample	Comments
22-01-2010 14-19-25	67	0.876	18.944	0.2	0	1	0	0				
22-01-2010 14-06-29	100	0.876	18.944	0.2	0	1	0	0				
22-01-2010 14-05-27	100	0.876	18.944	0.2	0	1	0	0				

ESRF | eLife | EMBL | DMLA | SPRING | MSD | eScience
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Data Exchange



ISPYB can be much more if you use it properly !

Lab Contacts

Search

New/Edit LabContact

Scientist name:

Scientist first name:

Select

Select the scientist contact

Scientist name	Scientist first name	Lab name	Action
TURKENBURG	J.P.	York Structural Biology Laboratory	<input type="button" value="Select"/>
LEONARD	Oorden	E S R.F.	<input type="button" value="Select"/>
MONACO	Stephanie	E S R.F.	<input type="button" value="Select"/>
TERRACOT-FROT	Laurent	E S R.F.	<input type="button" value="Select"/>
THIBAUT	Xavier	E S R.F.	<input type="button" value="Select"/>
SPRUCE	Darren	E S R.F.	<input type="button" value="Select"/>
GILJARD	Matias	E S R.F.	<input type="button" value="Select"/>
PIPELINE	Data	E S R.F.	<input type="button" value="Select"/>
CHA	Sunshin	Pohang Accelerator Laboratory	<input type="button" value="Select"/>
KIM	Inkwon	Department of Chemistry	<input type="button" value="Select"/>
KIM	Min-Kyu	Laboratory of Biophysics	<input type="button" value="Select"/>
AN	Young jun	Korea Ocean Research & Development Institute	<input type="button" value="Select"/>
SEO	Koung hye	Department of Chemistry	<input type="button" value="Select"/>
LEE	Kon ho	Gyeongang National University	<input type="button" value="Select"/>
KOSKI	Kristian	Department of Biochemistry	<input type="button" value="Select"/>
HAAPALAINEN	Antti	Department of Biochemistry	<input type="button" value="Select"/>
BUJACZ	Gazgor	Institute of Bioorganic Chemistry	<input type="button" value="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 status (if ESRF sends a device back):

Courier account:

Shipping reference:

Average Customs value of a device (Euro):





Average Transport value of a device (Euro):



Creating Shipments

Dewar Labels (sending, return)

Shipment Creation

New/Edit Shipment	
Details	
Creation date	2009-09-19
Shipment label	<input type="text" value="MyShipment"/>
Number of devices	<input type="text" value="2"/>
Number of other components (i.e. Boluses, Laser...)	<input type="text" value="1"/>
Baseline / Experiment	<input type="text" value="01-03-2009 D14 E 4"/>  <input type="text" value=""/> 
Comments	<input type="text" value="Thank!"/>
Shipment status	<input type="text" value="opened"/>
Lab contacts	
Lab-Contact for sending	<input type="text" value="MONACOE-S.R.F."/> 
Return address is identical as sending address (Y/N)	<input checked="" type="checkbox"/>
If No, Lab-Contact for Return	<input type="text" value="MONACOE-S.R.F."/> 

TO: **ESRF Magasin**
c/pt. Jules Horowitz
Orsay, Cedexexile
FRANCE
+33 1 69 15 16 212
+33 1 69 15 16 212
Fax: +33 1 69 15 16 217

From **Science in Sky Diploper**
 for **Experimentation 4200F**

Net: **notified**
 for **notified** **agence** **provision** **4202**

From **Science in Sky Diploper**
 for **Experimentation 4200F**

Net: **notified**
 for **notified** **agence** **provision** **4202**

FRANCE **Subsidiary** **working** **date**

Storage area **Initial**

Number of pieces **1**

From **1999**

Provenance **ESRF**

Acquisition date **1999**

Local control **Identification**

FRANCE **Subsidiary** **working** **date**

Storage area **Initial**

Number of pieces **1**

From **1999**

Provenance **ESRF**

Acquisition date **1999**

Local control **Identification**

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FRANCE **Subsidiary** **working** **date**

Storage area **Initial**

Number of pieces **1**

From **1999**

Provenance **ESRF**

Acquisition date **1999**

Local control **Identification**

FRANCE **Subsidiary** **working** **date**

Storage area **Initial**

Number of pieces **1**

From **1999**

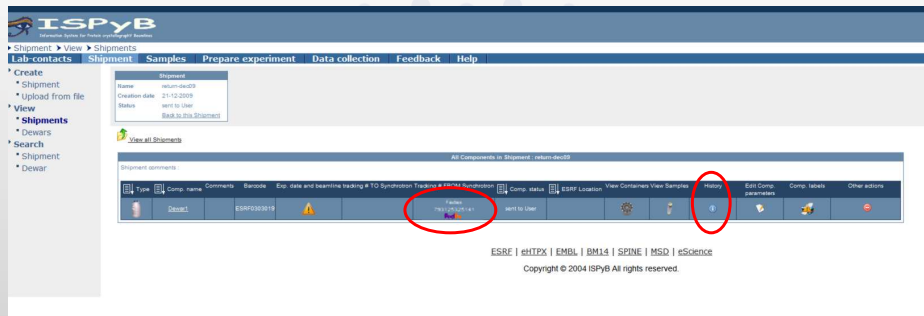
Provenance **ESRF**

Acquisition date **1999**

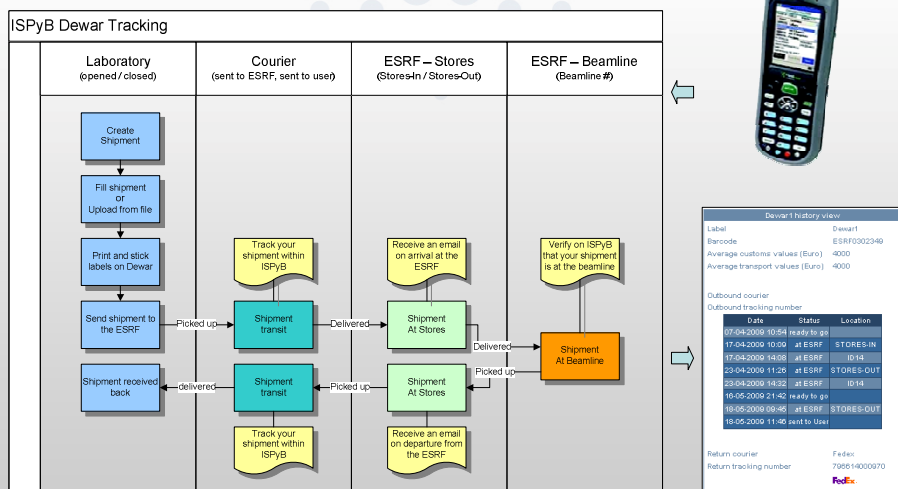
Local control **Identification**

Email sent when dewar arrives at stores and when it leaves !

From ISPYB link to Courier company



Dewar Tracking



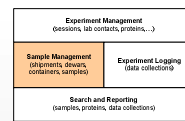
Sample Management

Items:

- Shipments (set of dewars)
- Dewars (barcode, courier tracking number)
- Containers (barcode)
- Samples (barcode, protein acronym, crystal form,...)

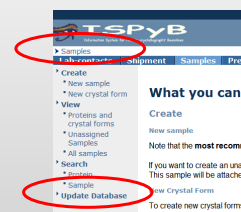
Features:

- Online shipment description
- Shipment description upload (Excel file)
- Dewar Tracking



How to get sample information into ISPYB

- Make sure that all sample sheets for the experiment have been submitted through SMIS and validated by safety.
- If sample sheets have recently been submitted you may need to update the database. Button found in Samples tab
- Create a Shipment
- Download a new excel sheet each time – the new sheet will have your newly submitted samples included
- Complete Excel sheets
- Upload information



Create a shipment

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Slide: 15

The more information you can provide the less chance of errors on the beamline.

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		ESRF	ESRF	ESRF															
3		ESRF	ESRF	ESRF															
4		ESRF	ESRF	ESRF															
5		ESRF	ESRF	ESRF															
6		ESRF	ESRF	ESRF															
7		ESRF	ESRF	ESRF															
8		ESRF	ESRF	ESRF															
9		ESRF	ESRF	ESRF															
10		ESRF	ESRF	ESRF															
11		ESRF	ESRF	ESRF															
12		ESRF	ESRF	ESRF															
13		ESRF	ESRF	ESRF															
14		ESRF	ESRF	ESRF															
15		ESRF	ESRF	ESRF															
16		ESRF	ESRF	ESRF															
17		ESRF	ESRF	ESRF															

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Slide: 16

In ISPYB make sure the correct dewar is activated

ISPYB
Instrument System for Protein Crystallography

Prepare experiment
Lab contacts Shipment Samples **Prepare experiment** Data collection Feedback Help

Select dewar
Fill sample changer
Select samples

Prepare your experiment:
1- Select the dewar you want for processing.
2- Fill the sample changer, assign a location for your containers (only required if not using Diamatrix codes)
3- In MxCuBE, link the samples in the container to the crystals in the Sample Changer.

Next step: Fill the sample changer

Note that the dewar shipments will be set in "processing" state and will not be editable any more.


Ship name	Creation date	Comp. name	Type	Comments	Barcode	Exp date	Dewar	# containers	Load	Dewar status	Location	View	View	History	Comp. labels	Select for processing
Test_crystal	17-12-2008	Dewar1			ESRF0102024		5 (50)		processing							Select
Test_crystal	17-12-2008	Dewar2			ESRF0102022		5 (50)									Select
demo	10-11-2008	Dewar1			ESRF001084	10-11-2008	2 (6)									Select
SQL_test	27-10-2008	Dewar1			ESRF001084	31-10-2008	1 (4)		THBAULT X	opened						Select
Oxide_Oxide	27-10-2008	Dewar2			ESRF001082	31-10-2008	5 (44)		THBAULT X							Select
Oxide_Oxide	27-10-2008	Dewar1			ESRF001082	31-10-2008	5 (45)		THBAULT X							Select
Bag Training	20-06-2008	None		Prepare Dewar for Bag Training			2 (25)									Select
effTXX		ESRF_A106.08					5 (46)		opened							Select
M-protein		Dewar1					4 (32)									Select
Mx2		Mx2					1 (4)									Select
CSP000144		AJA00014					1 (9)		opened							Select
mx15-R_20-2-2008		Dewar2					1 (4)									Select
mx15-R_20-2-2008		Dewar1					1 (4)									Select
mx15-R_20-2-2008		Dewar1					1 (10)									Select
mx15-R_20-2-2008		Dewar1					1 (10)									Select

Linking the information in ISPYB through mxCuBE

- **Use the barcodes:** Scan barcodes in Sample Changer mxCuBE will automatically match barcodes scanned in Sample changer with information in selected shipment.
- **If barcodes are not scanned correctly or if you are not using barcodes** – you can link the samples through ISPYB but be careful !

Link Samples

ISP Sample Changer





Information Systems for Protein crystallography facilities

- Prepare experiment
- Lab contacts Shipment Samples Prepare experiment Data collection Feedback Help**
- Select dewar
- Select sample changer
- Select samples

Prepare your experiment:

- Select the dewars you want for processing.
- Fill the sample changer: assign a location for your containers (only required if not using Damatrix codes)**
- In MxCuBE, link the samples in the container to the crystals in the Sample changer.

  **Next step: Link Samples in MxCuBe**

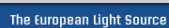
This step is not required if you are using Datamatrix code on your samples pins.

Containers to load in sample changer									
Shipment name	Shipment creation date	Dewar label	Dewar barcode	Container code	Container type	Container capacity	# samples	Barcode Location	Location in Sample Changer
Test crystals 2010	02-12-2009	Dewar1	ESRF0302972	AA414A	Puck	10	10	ID29	1
Test crystals 2010	02-12-2009	Dewar1	ESRF0302972	AA399A	Puck	10	10	ID29	2
Test crystals 2010	02-12-2009	Dewar1	ESRF0302972	AA382A	Puck	10	10	ID29	3
Test crystals 2010	02-12-2009	Dewar1	ESRF0302972	AA417A	Puck	10	10	ID29	4
Test crystals 2010	02-12-2009	Dewar1	ESRF0302972	AA373A	Puck	10	10	ID29	5

Save

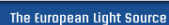
Makes life easier on the beamline.

[illegible]



Slide: 21

Especially if you have sample code names 98761954780



Slide: 22

Data Collections of a Session

Data Collections		Energy Scans												
Image Prefix	Run No	Protein Acronym	Start Time	# Images	Wavelength	Transm.	Ex. Time	Phi start	Phi range	Detector Resolution	Status	Sampling	Skip	Comments
All												Rank	Save	
Ins	2		08-07-2009 17:15:58	14	0.976	100	0.34	115.95	0.3	1.54	<div><div></div><div></div><div></div><div></div><div></div></div>	<div><div></div><div></div><div></div></div>	<div><div></div><div></div></div>	
Ins	1		08-07-2009 17:14:03	57	0.976	100	0.1	96	0.35	1.54	<div><div></div><div></div><div></div><div></div><div></div></div>	<div><div></div><div></div><div></div></div>	<div><div></div><div></div></div>	
ref-ins	2		08-07-2009 17:05:01	2	0.976	100	1	0	1	1.5	<div><div></div><div></div><div></div><div></div><div></div></div>	<div><div></div><div></div><div></div></div>	<div><div></div><div></div></div>	Collecting 2 reference images
ref-ins	1		08-07-2009 16:54:21	2	0.976	100	1	0	1	1.7	<div><div></div><div></div><div></div><div></div><div></div></div>	<div><div></div><div></div><div></div></div>	<div><div></div><div></div></div>	Collecting 2 reference images
FAE-XSS	4		08-07-2009 14:42:52	21	0.976	100	0.65	112.95	0.5	1.7	<div><div></div><div></div><div></div><div></div><div></div></div>	<div><div></div><div></div><div></div></div>	<div><div></div><div></div></div>	
FAE-XSS	3		08-07-2009 14:41:33	31	0.976	100	0.4	92.8	0.65	1.7	<div><div></div><div></div><div></div><div></div><div></div></div>	<div><div></div><div></div><div></div></div>	<div><div></div><div></div></div>	
FAE-XSS	2		08-07-2009 14:40:39	22	0.976	100	0.31	63	0.9	1.7	<div><div></div><div></div><div></div><div></div><div></div></div>	<div><div></div><div></div><div></div></div>	<div><div></div><div></div></div>	

Parameters & Results

Input parameters	Resulting parameters	SWA results
Input directory	/data/colloc/2010/4250/4250-44/20090919/540	
Input prefix	star-fid	
Star size	3	
Start Time	09-09-2009 11:27:53	
End Time	09-09-2009 11:39:01	
Type of experiment		
WaveLength	0.3796 Å	
Energy	12,456 eV	
Phi start	167.0°	
Displacement-range	0.75°	
Scanning	0.5°	
Exposure Time	0.5 s	
Number of passes	1	
Detector Distance	293.5 mm	
Resolution at edge	1.9 Å	
Resolution at center	1.52 Å	
Slitless	155.72 mm	
Slitless	156.91 mm	
Detector Slitless	0.5	
Kappa	90 Å	
Phi	90 Å	

Data Analysis reports

```

Distance From 0 Mile collection
Remission Time (hr) to 0 Mile to the next Mile time
Atmosphere = 0.000000
M1 PM2.5 at 0.1 mppm (hr weight Exposure) Distance (km)
1 182.68 62% 0.20 0.43 250.0 1
Remission time (hr) 1
Sample size 2
PM2.5 at 0.1 mppm 0.43
Total station time 182.68
Total # of samples 2
Number of Collections 1
Q-factor (none used) 0
Coversure cover small 1
Q-factor 0
Total Data Collection time 2
Data collection statistics
Group Name n Group Mean Group SD
Remission Time 2
182.68 62 921.98975 1.879438
0.20 4 94.76364 7.932616
0.43 80 32.13085 2.7712
0.62 16 30.82377 3.68804
0.75 16 30.55046 3.0000

```

Crystal Snapshots

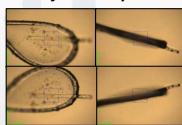
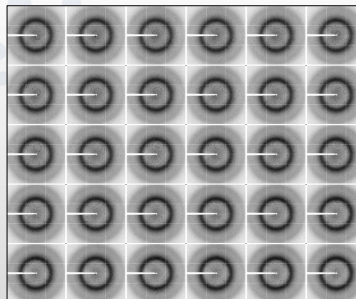
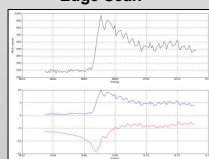


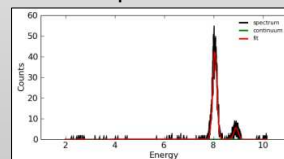
Image thumbnails (image wall)



Edge Scan



XRF Spectrum



Search and Reporting

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

Search

- Data Collection records (protein, sample, experiment date,...)
- Proteins
- Samples

Reports: Usually as data collection sessions

- Data collection lists – pdf
- Screening – pdfs & Word documents
- CSV for import into other LIMs

Search

Protein or Sample

Search Protein

Acronym

Project	System Group	Sample	Temp	Platform	Device	Language	Loc	Test Case ID	Test Case Name	Code	Ready	Result	Sample	Editor	Sample	Date
FAC	P210721	5467	5000000000	2018-10-01-0000	Net Group	C#(MS)	1	MS-100-1113	MS-100-1113	MS-100-1113	0	0	0	MS-100-1113	MS-100-1113	2018-10-01-0000
FAC	P210721	5468	5000000000	2018-10-01-0000	Net Group	C#(MS)	2	MS-100-1113	MS-100-1113	MS-100-1113	0	0	0	MS-100-1113	MS-100-1113	2018-10-01-0000
FAC	P210721	5469	5000000000	2018-10-01-0000	Net Group	C#(MS)	3	MS-100-1113	MS-100-1113	MS-100-1113	0	0	0	MS-100-1113	MS-100-1113	2018-10-01-0000
FAC	P210721	5469	5000000000	2018-10-01-0000	Net Group	C#(MS)	4	MS-100-1113	MS-100-1113	MS-100-1113	0	0	0	MS-100-1113	MS-100-1113	2018-10-01-0000
FAC	P210721	5469	5000000000	2018-10-01-0000	Net Group	C#(MS)	5	MS-100-1113	MS-100-1113	MS-100-1113	0	0	0	MS-100-1113	MS-100-1113	2018-10-01-0000
FAC	P210721	5467	5000000000	2018-10-01-0000	Net Group	C#(MS)	6	MS-100-1113	MS-100-1113	MS-100-1113	0	0	0	MS-100-1113	MS-100-1113	2018-10-01-0000
FAC	P210721	5468	5000000000	2018-10-01-0000	Net Group	C#(MS)	7	MS-100-1113	MS-100-1113	MS-100-1113	0	0	0	MS-100-1113	MS-100-1113	2018-10-01-0000
FAC	P210721	5469	5000000000	2018-10-01-0000	Net Group	C#(MS)	8	MS-100-1113	MS-100-1113	MS-100-1113	0	0	0	MS-100-1113	MS-100-1113	2018-10-01-0000
FAC	P210721	5469	5000000000	2018-10-01-0000	Net Group	C#(MS)	9	MS-100-1113	MS-100-1113	MS-100-1113	0	0	0	MS-100-1113	MS-100-1113	2018-10-01-0000
FAC	P210721	5467	5000000000	2018-10-01-0000	Net Group	C#(MS)	10	MS-100-1113	MS-100-1113	MS-100-1113	0	0	0	MS-100-1113	MS-100-1113	2018-10-01-0000

Data Collection

Search data collection

Sample name:

Protein acronym:

Beamline:

Experiment data 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	Image Refs	Run No	Protein Accession	Start Time	# Images	Wavelength	Transm.	Distance	Ex. FWHM	Pin. start range	Beam Y-axis	Detector Resolution	Status	Sample Name	Comments		
			FAE											Rank			
	FAE001	3	FAE	08-07-2009 13:26:14	209	0.976	100	211.7	0.07	67	0.45	159.159.165.34	1.62		■	DNA data collected	
	FAE002	2	FAE	08-07-2009 13:26:19	2	0.976	100	226.01	1	0	1	159.18.165.36	1.7		■	Collecting reference image	
	FAE003	1	FAE	08-07-2009 13:00:25	1	0.976	100	226.1	0	0	1	159.16.165.36	1.7		■	Collecting reference image	
	test1	2	FAE	19-08-2009 16:49:03	1	0.873	100	204.72	1	0	1	112.55.112.14	4		■		
	test2	1	FAE	19-08-2009 16:49:03	1	0.873	100	60.72	1	0	1	112.55.112.14	4		■		
	FAE004	1	FAE	19-08-2009 13:11:41	1	0.873	100	134.32	1	0	1	112.42.112.11	5		■		
	FAE005	1	FAE	01-04-2009 19:47:41	1	0.903	100	239.8	1	0	1	96.4	95.45	3.13		■	
	FAE006	2	FAE	01-04-2009 19:47:41	103	0.903	178.61	160.7	0.05	151	0.7	96.47	95.38	1.97		■	DNA data collected
	test3	2	FAE	01-04-2009 15:00:25	3	0.903	100	178.61	0.07	241	0.7	96.47	95.38	1.97		■	
	FAE007	4	FAE	01-04-2009 14:55:22	2	0.903	100	186.1	0	0	1	96.47	95.39	2		■	Collecting reference image
	FAE008	1	FAE	01-04-2009 14:55:22	2	0.903	2.1	183.95	1	0	1	96.47	95.39	2		■	Collecting reference image

Reporting

Pdf

Word

Pdf

Excel / Csv

The European Light Source

Slide: 27

DNA & EDNA characterisation

EDNA & EDNA characterisation

File Edit View Help Settings About

Process Results

Available samples:

Name	Acronym	Barcode	Location	Space group	a b c α β γ	Mt.res.	Basket
typex15	typ	H400A0N78	1.02	P2 ₁ 2 ₁ 2 ₁	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex17	typ	H400A0N79	1.01	P2 ₁ 2 ₁ 2 ₁	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex18	typ	H400A0S077	1.04	P2 ₁ 2 ₁ 2 ₁	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex19	typ	H400A0N88	1.05	C23	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex13	typ	H400A0N87	1.06	C23	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex14	ns	H400A0S084	1.07	C23	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex1y05	TLN	H400A0N82	1.02	Pn32	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
thermox106L	TLN	H400A0S077	1.09	Pn32	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
thermox107	TLN	H400A0S078	1.10	Pn32	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
SatMx103	FAC	H400A0S081	2.01	P2 ₁ 2 ₁ 2 ₁ C4 S12 B 11.9 90.0 90.0 90.0	0.0		
typex12	typ	H400A0N75	2.02	P2 ₁ 2 ₁ 2 ₁	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex11	typ	H400A0N74	2.01	P2 ₁ 2 ₁ 2 ₁	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex14	typ	H400A0N76	2.04	P2 ₁ 2 ₁ 2 ₁	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex15	typ	H400A0Q89	2.05	P2 ₁ 2 ₁ 2 ₁	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex16	ns	H400A0N89B	2.06	C23	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex10	ns	H400A0S080	2.07	C23	0.0 0.0 0.0 0.0 0.0 0.0	0.0	
typex1	ns	H400A0S083	2.08	C23	0.0 0.0 0.0 0.0 0.0 0.0	0.0	

☒ Show only the samples inside the sample changer (20 samples)

Group by: no grouping Refresh

Directory: [data:\home\c15\141-AH-02\020\FAZ\SatMx1AE1] Browse Prefix: FAZ-SatMx1AE1 Run number: 1

☒ 1st step: Take reference images
Template: [data:\home\c15\141-AH-02\020\FAZ\SatMx1AE1\FAC-SatMx1AE1_1_#ref.img]
Oxidation range (deg): 1.0 Exposure time (s): 1.0 Screening resolution (Å): 2.00

☒ 2nd step: Index reference images
Template: [data:\home\c15\141-AH-02\020\FAZ\SatMx1AE1\FAC-SatMx1AE1_1_#ref.img] Browse

Space group: unknown

☒ 3rd step: Calculate strategy
Max-resolution (deg): Multiplicity: Anomalous: ☐

☐ 4th step: Collect data
Data file: [data:\home\c15\141-AH-02\020\FAZ\SatMx1AE1\FAC-SatMx1AE1_1_#.h5] Save
Start angle: On start (min) (deg) Exposure time (s) Image size (pixels)
Rotational angles: On start (min) (deg) Rotation (°) Rotations per exposure

d's d's
Execute steps: [http://www.diamond.ac.uk/edna/] OK Cancel

Information messages | Submit feedback | Chat CB | Open Book | EDNA Log

Current results:
Machine current: 181.7 mA
X-ray: 150.0 kV
Cryo: 100.0 %
Dry: unknown
Superflying: unknown
Collect stage: unknown
Phasing beamline: unknown
Mounting sample: unknown
Centring sample: unknown
Collecting images: unknown
I/O flux: 0 photons

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Slide: 28

European Synchrotron Radiation Facility

Lab-contacts
Shipment
Samples
Prepare experiment
Data collection
Feedback
Help

View last sessions
View all sessions
Search data collections

Selected Sample

Name: X21

[Sample details](#)

Selected Session

Start Date: 20-10-2009

BeamLine: ID14.4 +33470982322

[Back to this session](#)
[Back to sessions](#)

Selected DataCollection

Start Time: 20-10-2009

Image Prefix: refFAE/X21

Run Number: 1

[Back to this data collection](#)

Experiment parameters

Beamline parameters

DNA results

Main output parameters:

Indexing status: Indexing successful
Spacegroup: P222
Unit Cell a: 65.81 Å
Unit Cell b: 108.934 Å
Unit Cell c: 113.576 Å
Unit Cell alpha: 90.0 °
Unit Cell beta: 90.0 °
Unit Cell gamma: 90.0 °
Mosaicity: 0.25 °
Resolution observed: 1.38 Å
I/Sig at that resolution: 3.0
Number of spots used: 3124
Number of spots total: 3710
Spot deviation angular: 0.112745
Spot deviation positional: 0.114547
Beam shift x: -0.114547
Beam shift y: 0.053894
Predicted resolution (BEST): 1.22

DNA output files:

DNA characterisation & strategy
Ranking summary
dna_log.txt
mosfm-integrate log
pointless log
scale log

DNA strategies

Phi	Start	Phi	End	Rotation	Exposure	Time	Strategy	Resolution	Total exposure	Time	Total	Nb images	Program	Program log file
21.0	116.4	0.6	0.0	1.79	8.0	159	BEST 3.1.0c						View BEST_log file	
21.0	116.4	0.6	0.0	1.79	8.0	159	User defined strategy used for data collecti							

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Slide: 29

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Sample Ranking

Ranked Samples

Sample Screening

DNA/EDNA Characterisation

Sample Ranking & Selection

Data Collect

...

Selected Sample

Image Prefix

Run No

Start Time

Space Group

UC a

UC b

UC c

Ranking resol

Exposure time s

Mosaicity

Number of spots

Number of images

Total

WT	WT	WT	WT	WT	WT	Rank
<input checked="" type="checkbox"/>	refP2-35b112	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"/>	refP2-7_dna	1	15:31:14	P4	66 68 101	#1 1.99 #4 547.5 #2 0.53 #6 1107 #2 61 #2 70 %
<input checked="" type="checkbox"/>	refDNAH000A00096	1	16:09:47	P222	65 126 230	#8 3.08 #9 604.0 #8 0.72 #13 510 #1 48 #3 68 %
<input checked="" type="checkbox"/>	refP2-35b0-1	4	11:25:50	P2	74 107 102	#10 3.34 #10 618.3 #1 0.48 #10 775 #5 80 #4 87 %
<input checked="" type="checkbox"/>	refmfe1111b	1	20:10:36	P222	65 126 228	#5 2.85 #3 470.8 #2 0.53 #11 755 #7 98 #5 67 %
<input checked="" type="checkbox"/>	refP2-35b0-1	1	10:19:09	P2	74 107 102	#7 2.99 #6 585.1 #9 0.74 #7 1100 #3 70 #6 66 %
<input checked="" type="checkbox"/>	refmfe1100b	1	20:34:00	P222	65 126 230	#3 2.81 #2 386.0 #5 0.62 #4 1269 #13 830 #7 52 %
<input checked="" type="checkbox"/>	refP2-35b0-1	2	10:38:23	P2	74 107 102	#9 3.12 #11 631.4 #10 0.82 #9 845 #4 74 #8 51 %
<input checked="" type="checkbox"/>	refP2-35b0	1	10:26:32	P2	74 107 102	#10 3.34 #13 647.5 #7 0.70 #5 7129 #6 98 #9 51 %
<input checked="" type="checkbox"/>	refmfe1189b	2	20:35:55	P222	65 126 230	#4 2.84 #8 697.4 #5 0.62 #3 1559 #11 760 #10 50 %
<input checked="" type="checkbox"/>	refDNAH000A01704	1	16:06:19	P222	65 126 230	
<input checked="" type="checkbox"/>	refmfe1100b16-11	1	16:13:16	P222	65 126 230	
<input checked="" type="checkbox"/>	refP2-35b0-2	1	10:23:13	P2	74 107 102	

Ranking Chart

Sample List

Colour	Select	Rank	Year	Image prefix	Sp	Ni
<input checked="" type="checkbox"/>	3	79	refP2-35b112	C-1	2	
<input checked="" type="checkbox"/>	3	64	refP2-35b0-1	P-1	1	
<input checked="" type="checkbox"/>	3	51	refmfe187	P-1	1	
<input checked="" type="checkbox"/>	4	54	refmfe181b	P-1	1	
<input checked="" type="checkbox"/>	5	54	refmfe181b	P-1	1	
<input checked="" type="checkbox"/>	4	53	refmfe181b	P-1	1	
<input checked="" type="checkbox"/>	7	52	refmfe181b	P-1	1	
<input checked="" type="checkbox"/>	8	53	refmfe181b	P-1	1	
<input checked="" type="checkbox"/>	9	52	refmfe181b	P-1	1	
<input checked="" type="checkbox"/>	10	51	refP2-35b0-1	P2-1	1	
<input checked="" type="checkbox"/>	11	51	refmfe181b	P-1	1	
<input checked="" type="checkbox"/>	12	50	refP2-35b0-1	P2-1	1	
<input checked="" type="checkbox"/>	13	50	refP2-35b0-1	P2-1	1	
<input checked="" type="checkbox"/>	14	50	refmfe181b	P-1	1	
<input checked="" type="checkbox"/>	15	49	refmfe181b	P-1	1	
<input checked="" type="checkbox"/>	16	47	refmfe181b	P-1	1	
<input checked="" type="checkbox"/>	17	47	refmfe181b	P-1	1	
<input checked="" type="checkbox"/>	18	47	refDNAH000A01704	P-1	1	
<input checked="" type="checkbox"/>	19	46	refP2-35b0-1	P2-1	1	

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Slide: 30

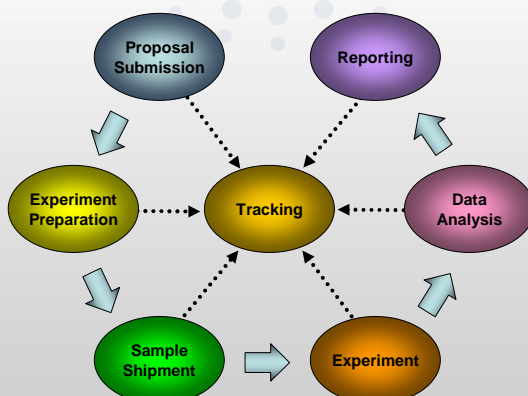
Ranking

Information from ranking can be used to direct further data collections

We are working on automatic ways of doing this...

In the future - Samples selected through ISPYB will be automatically loaded by the sample changer, centered using play-back centering and collected through mxCuBE.

From your sample to your data analysis and then back again !
Sample Tracking, screening and further data analysis.



Current & Planned Developments

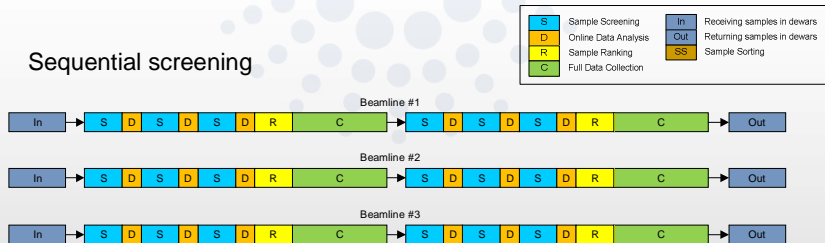
- Extend to include EDNA characterisation as well as DNA
- Extend to include downstream Data processing statistics
- Linking snapshots in ISPYB for playback centering
- Data presentation/ visualisation. Move from Session > Project view

The Future Plans

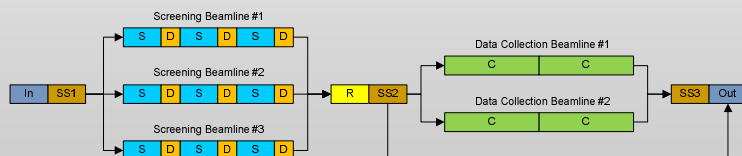
- ISPyB and UPBL10/MASSIF
- ISPyB for BioSAXS (ID14-3)
 - ISPyB for other beamlines
- ISPyB for other MX facilities

ISPyB and UPBL10/MASSIF : extreme sample tracking

Sequential screening



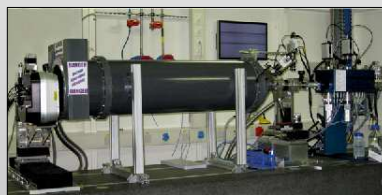
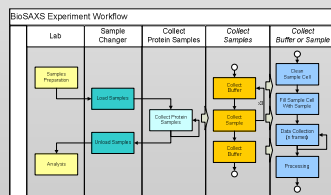
Dedicated screening beamlines and then ranking and sorting of samples for data collection on other beamlines



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: how does it help?

The Users

- Prepare Experiment at home not on the beamline
- Remote tracking by colleagues at home while the experiment is performed
- Information from ISPYB can be exported into the home labs database
- Long term tracking of experiments

ESRF Staff (Including Data collection staff)

- Improved communication between Users and ESRF Staff
- 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

Everyone knows where the dewars are at any time !

ISPyB: how does it help?

Managements and Operations

- Dashboards for monitoring operations
- Statistics on how experiments are carried out
 - Screenings/Full data collections ratio,...
 - Figures on feature usage (training, interface improvement...)
 - Figures on data throughput (Data Collection Pipeline optimization)

Safety Like

- Sample Tracking

How can we help ?

Send questions, comments and suggestions:

ispyb@esrf.fr