



| The European Synchrotron

What is ISPyB ?



Solange Delagenière, MIS group, ESRF

What:

ISPYB is a Laboratory Information Management System (LIMS) linking samples to their corresponding data. It is based on a dynamic web application using a MySQL database.

How:

Access to ISPYB? <http://ispyb.esrf.fr>

To log-in: user account or experiment account

Why:

it has taken a more important role over the years : to face the deluge of data coming from our detectors, to keep and exploit metadata

MX: ~2K data collections from MX beamlines in 2005, ~ 107K in 2013

Bx: 980K frames collected, 26K data collections done, 1170 HPLC, 4186 Sample Changer

What is ISPyB?

History

2001 - 2005: Pxweb (experiment reporting only).....



2005 - 2009: ISPyB (experiment reporting & much more)

Collaborations



2012: BioSAXS extension:

Collaboration between ESRF, EMBL HH & DLS

2014: collaboration with SOLEIL : Gentleman's Agreement, EMBL, MAX lab.....



Where are we today ?

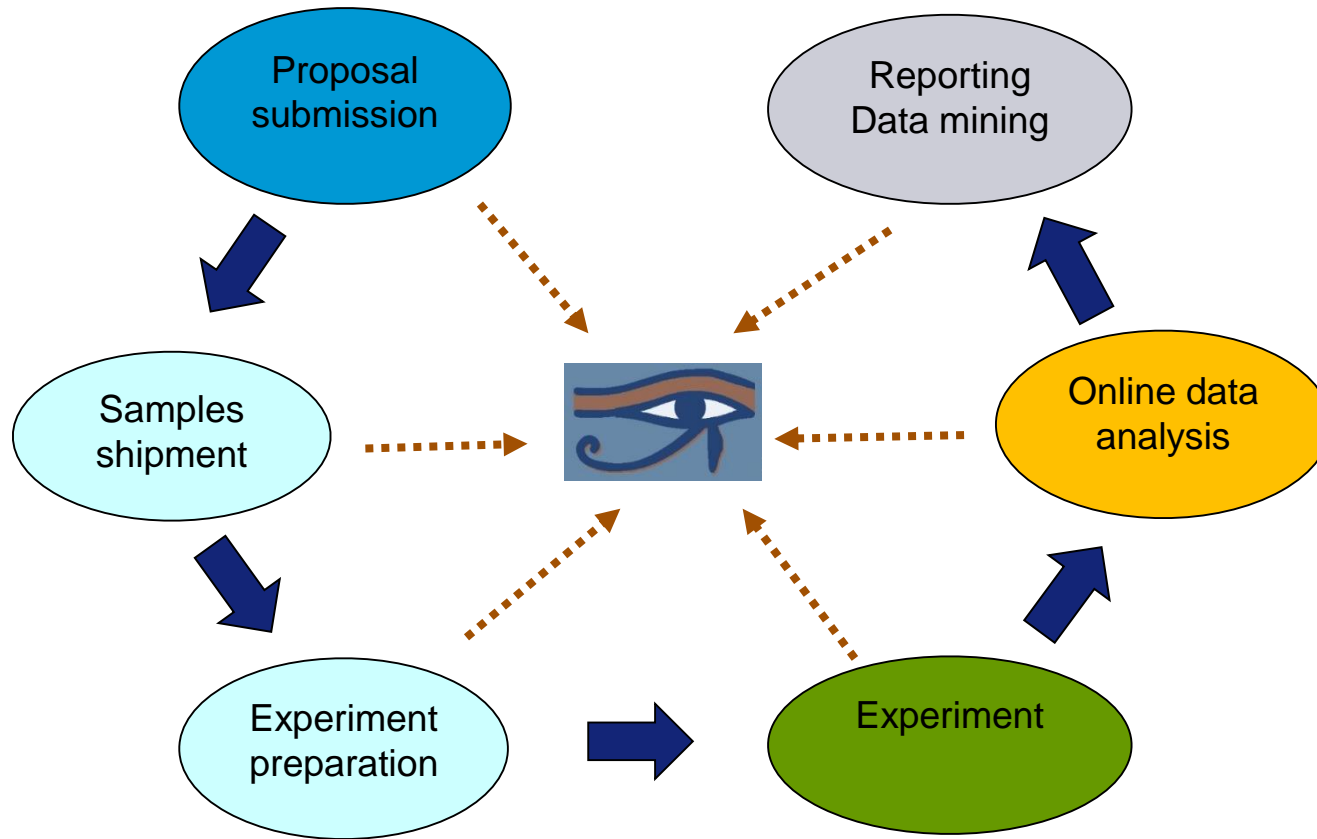
• Current ISPyB & ISPyBB version :



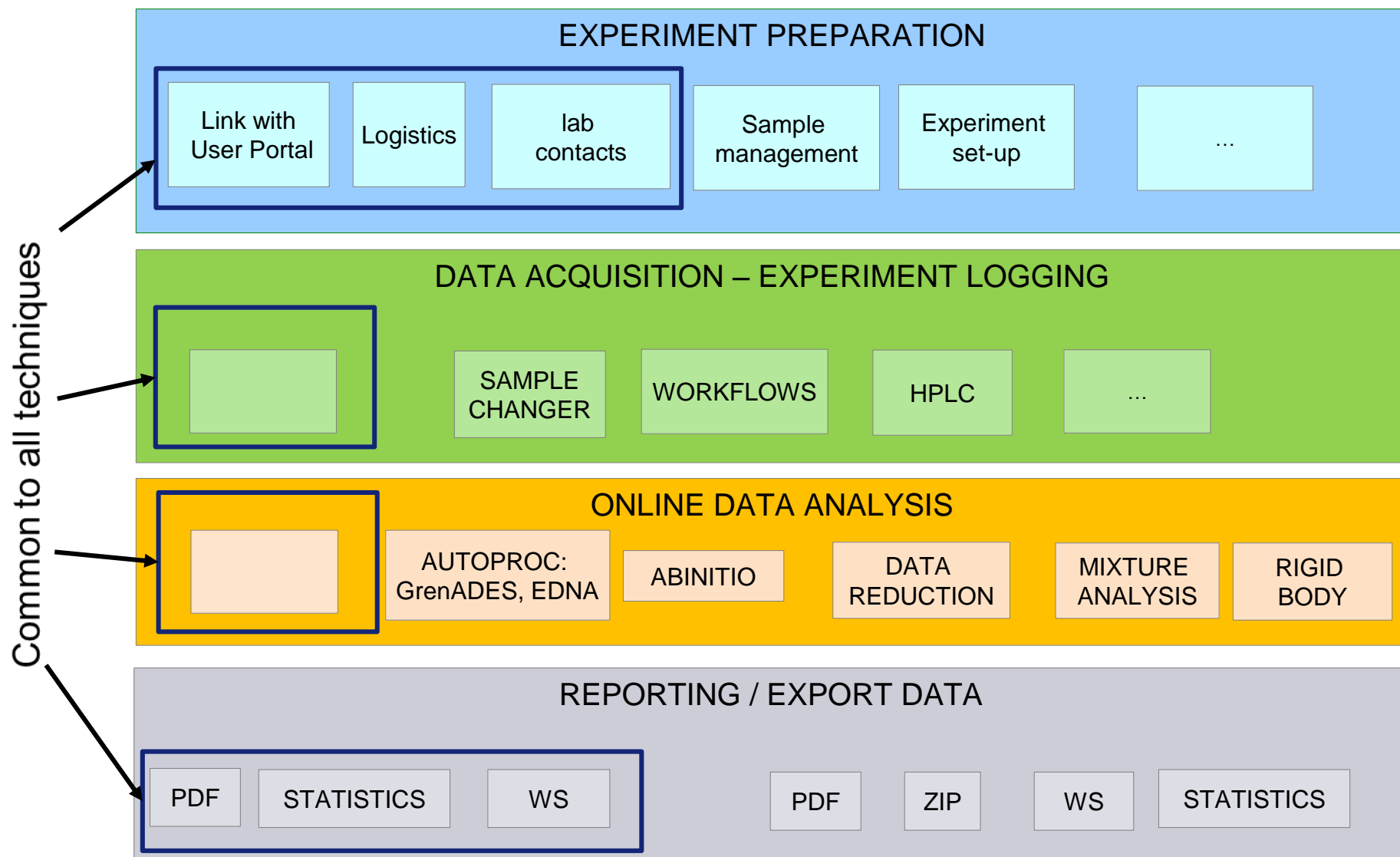
• Other ISPyB versions : synchweb, synchlink; ISPyBB (2013); old ISPyB MX (2010)



What is ISPyB : a Laboratory Information Management System



ISPyB Features & Modules



What is ISPyB : let's log in

ISPyB
Information System for Protein crystallography Beamlines

Help | **Logon**

- ▶ **ISPyB Overview**
- ▶ **Latest ISPyB News**
- ▶ **References**
- ▶ **Get Firefox**
- ▶ **Need help**

Login	Messages
<p>Login</p> <input type="text"/> <p>Password (*)</p> <input type="password"/> <p>(*): Your beamline proposal password is now randomly generated. You can retrieve this password from your A-form, login to the ESRF User Portal webclient here.</p> <p><input type="button" value="Login"/> <input type="button" value="Reset"/></p>	<p>If you want to subscribe to the ISPyB-news mailing list, click here.</p> <p>If you encounter any problems within ISPYB please contact us at ispyb@esrf.fr.</p> <p>Please note that for maintenance purposes, ISPYB may be stopped every MDT Day (Machine Dedicated Time), usually Tuesday, at any time between 10am and noon.</p>

[ESRF](#) | [EMBL](#) | [BM14](#) | [SPINE](#) | [MSD](#) | [Diamond](#) | [SOLEIL](#) | [EMBL](#) | [MAXIV](#)

Copyright © 2004 ISPyB All rights reserved.

What is ISPyB : let's log in



Help

- ▶ ISPyB Overview
- ▶ Latest ISPyB News (@esrf)
- ▶ References
- ▶ Get Firefox
- ▶ Need help

Login	Messages
<p>Login</p> <p><input type="text" value="albnar"/></p> <p>Password (*)</p> <p><input type="password" value="*****"/></p> <p>(*): Your DUO password. Only when you have registered your beam time in the DUO system you will be able to add sample information. Beam line personnel will have to grant you access after registration (email mx@maxlab.lu.se).</p> <p><input type="button" value="Login"/> <input type="button" value="Reset"/></p>	<p>Please note that for maintenance purposes, ISPyB may be stopped every MDT Day (Machine Dedicated Time), usually Monday, at any time between 8am and noon</p>



[ESRF](#) | [EMBL](#) | [BM14](#) | [SPINE](#) | [MSD](#) | [Diamond](#) | [SOLEIL](#) | [EMBL](#) | [MAXIV](#)

Copyright © 2004 ISPyB All rights reserved.



Welcome

Select the proposal you want to work on :

Proposals			
Proposal	Title	Type	
☰ SAXS			
MX415	TEST	SAXS	GO
☰ MX			
IN906	Analysis of strain and Ge concentration on electronic substra...	MX	GO
IN832	EDDAM project	MX	GO
IN679	XRT on various foods products	MX	GO
IN905	3D characterization of a catalytic membrane based on PLI an...	MX	GO
MX415	TEST	MX	GO
MX410	TEST PROPOSAL FOR CS-MIS GROUP	MX	GO

1

1. Log in to SUN set (User Office web application) with user credentials

 Access to all proposals of connected user with given role(s)

2. Click on proposal number that you want to run in ISPyB

 Log on ISPyB successfully by means of servlet filter

 No regression in the code

 direct log on with proposal credentials is still possible

3. Automatic redirection to ISPyB
(no need to enter again credentials)

Note:

to embed

Any facility involved can make use of this feature






2



How to submit | Preparing your experiment | Laboratories support facilities | Safety requirements | Beamlines | User Office









- Home
- Proposal Management
 - Proposals list
- Experiment data
- SOLEIL Data Retrieval
- Personal Management
- User functions
- About
- LogOff


Proposals List

Enter search string here ... || Filter  ||     Default ▾


Status : Accepted Declined DIR Review Finished PRC Review Submitted Editing

Total Nb of props: 2

 Create ▾  Help ||   1-2 of 2  20  ||  Export  Add Columns

Proposal ID	General title	BAG coordinator or main proposer	1st Beamline Requested / Assigned	Status	Type	Safety
20130034	Observation of Total SUN Eclipse @ SOLEIL	Mr. CHADO Idrissou	PROXIMA 1	Editing	TransNational Access_EU	
20100077	Butterfly effect inside ISPyB	Mr. CHADO Idrissou	SWING	Accepted	Standard	

Connected as: CHADO Idrissou - Time: 2015/03/23 - 11:18



Logoff bx20100077 (Mr. Idrissou CHADO)
TEST SERVER on LOCAL

Home | Lab-contacts | **Shipping** | Prepare Experiment | Data Acquisition | Explore Your Results | Feedback | Help | Logoff

Welcome to User : bx20100077

In case of problems when creating shipments/samples, update ISPyB database (this may take a few minutes).

Shipping Tab

Click on this tab to deal with the samples you are planning to send by courier.
You will be able to:
Define an shipment, containing stock solutions and cases
You will be able to retrieve information about the shipments and cases

Currently your proposal contains:
0 Stock Solutions
0 Shipments

Prepare Experiment Tab

Click on this tab to deal with data concerning your samples
You will be able to:
Create new samples for experiment: samples description will be based on the protein you have submitted through "samplesheets".
Define the buffers you plan to use for data collection
Program data collections with the sample changer

Currently your proposal contains:
11 Macromolecules
0 Buffers
0 Exp. Templates

Data Acquisition Tab

Click on this tab to deal with the data collection you perform on your samples
You will be able to:
Retrieve information about a particular session
Retrieve information about a particular data collection
Retrieve information about a particular session
Retrieve information on the results from the data analysis pipeline

Currently your proposal contains:
2 Sessions
0 Calibration
0 Static. Exp.
0 HPLC Exp.

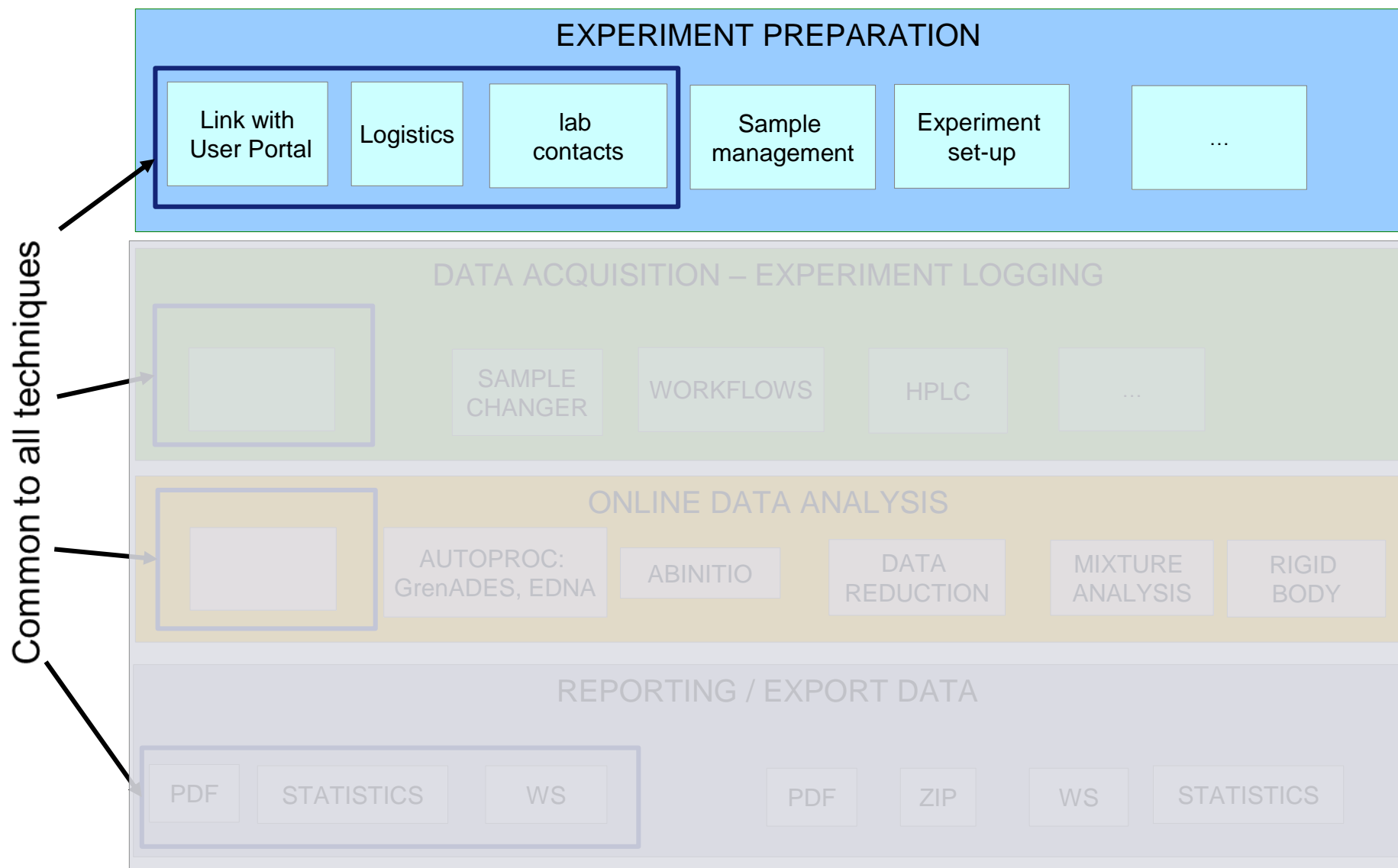
Explore your results

Click on this tab to deal with the data collected for your macromolecules
You will be able to:
Find all data collections you did for a macromolecule and an estimate of their quality
Compare results from different collections and sessions

Currently your proposal contains:
0 Data Collections

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

ISPyB Features & Modules



What is ISPyB : creating and filling in shipments

Upload from Excel, or csv

Samples & shipments

Lab contacts

Create shipment

New/Existing Shipment

Creation date: 2008-05-10

Shipment label: MyShipment

Number of devices: 2

Number of other components (i.e. Resonator, Laser...): 1

Beamline / Experiment: 15BMD01-01

Comments: 15BMD01

Shipment status: issued

Lab contacts: Labcontacts

Lab-Contact for sending: MONACO@ESRF

Lab-Contact for return: MONACO@ESRF

Return address is identical to sending address (Y/N)

Save

Puck Information

Shipping: ship-20131202

Dewar: Dewar1

Puck: Puck1

Create Puck

Save Reset Change sample name automatically

Sample Position	Protein Acronym	Space Group	Sample Name	Pre-Observed resolution	Needed resolution	Oscillation Range	Experiment Type	Unit Cell a	Unit Cell b	Unit Cell c	Unit Cell alpha	Unit Cell beta	Unit Cell gamma
1	tryp - P2	P2	sample01	0	0	0	Default	0	0	0	0	0	0
2	t2 - P21	P21	sample02	0	0	0		75.6	107	101.9	90	103	90
3	F4H - Undefined		sample03										
4	P4H - C2		sample04				OSC						
5	PDIM20 - Undefined		sample05				OSC						
6	pfk - P6122		sample06				OSC						
7	Prot_K - P43212		sample07				OSC						
8	RBCX - Undefined		sample08				OSC						
9	SAHase - Undefined		sample09				OSC						
10	SCPX - Undefined		sample10				OSC						
	SeDJ-1 - Undefined												
	SMhAG3 - Undefined												
	SOD - Undefined												
	t2 - C222												
	t2 - Undefined												
	t2 - P21												

or fill on line

ESRF | eHTPX | EMBL | BM14 | SPINE | MSD | eScience

Copyright © 2004 ISPyB All rights reserved.

EXPERIMENT PREPARATION

What is ISPyB : creating/retrieving lab-contacts

EXPERIMENT PREPARATION



Lab-contacts > Create > LabContact

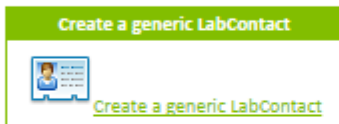
Home | References | Lab-contacts | Shipment | Samples | Prepare experiment | Data collection | Feedback | Help

- ▶ Create
 - LabContact
- ▶ View
 - LabContacts

Shipments & samples

Lab contacts

Logistics
Dewar tracking



New/Edit LabContact

Scientist name

Scientist firstname

LabContact > Lab-contacts | Shipment | Samples | Prepare experiment | Data collection | Feedback

- (Informations retrieved from ISPYB database)

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

Courier accounts details for return

These informations are relevant for all shipments.

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

Courier account

Billing reference

Average Customs value of a dewar (Euro)

Average Transport value of a dewar (Euro)

Max IV : created in DB

ESRF, EMBL, SOLEIL : retrieved from SMIS

Shipments/samples

Dewar location tracking

Communication between users / ESRF staff

Lab contacts

Dewar description (beamline, local contact, user address)

Labels automatically filled in

Logistics :
Dewar tracking

Automatic email on arrival / departure at / from the ESRF store

TO: ESRF Magasin
6 rue Jules Horowitz
38042 Grenoble
FRANCE
Tel: +33 (0)4 76 88 2733
+33 (0)4 76 88 7352
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	bShipTest
Number of parcels	1
Proposal number	MX115
Beamline	ID23-1
Experiment date	29-01-2013
Local contact	MONACO S

FROM : (Lab-contact sending)
MONACO Stéphanie
E.S.R.F.
6 rue Jules Horowitz
B.P. 220
F-38043 Grenoble Cedex
France
Tel: 33 (0)4 76 88 20 04 Fax:

Dewar1 history view		
Label	Dewar1	
Barcode	ESRF0307711	
Average customs values (Euro)	50	
Average transport values (Euro)	50	
Outbound courier		
Outbound tracking number		
Date	Status	Location
03-03-2015 11:06	ready to go	
05-03-2015 15:15	at ESRF	BM30
06-03-2015 08:16	processing	
09-03-2015 14:16	ready to go	
09-03-2015 14:18	ready to go	
10-03-2015 10:26	sent to User	
Return courier		
Return tracking number		
	DHL	
	9111235954	

Dear User,

Your parcel **Dewar3** (Proposal: **MX1689**, Session date: **16-03-2015**, Shipment: **MX1689_ID30A-3_160315**, Barcode: **ESRF0307753**) has left the ESRF and has been sent to your lab by **TNT** (Tracking Number: [987507323](#)) on 18/03/2015 at 1:40 PM (GMT+0100).

Don't hesitate to contact us at dewar-stores@esrf.fr if you encounter problems with its transport.

Best regards

The ESRF stores

Shipments & samples

Lab contacts

Logistics

Experiment Set up

Prepare your experiment:

- 1- Select the dewars you want for processing.
- 2- Fill the sample changer: assign a location for your containers (only required if not using Damatrix codes)**
- 3- 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	Beamline Location	Location in Sample Changer
ship-20141114	14-11-2014	Dewar1		MASSIFSAD	Puck	10	5	ID30A-1 ▾	16 ▾
ship-AR	03-09-2014	Dewar1	ESRF0306914	puckMD	Puck	10	10	ID23-1 ▾	1 ▾
ship-AR	03-09-2014	Dewar1	ESRF0306914	PuckMeike	Puck	10	10	ID23-1 ▾	4 ▾
ship-AR	03-09-2014	Dewar1	ESRF0306914	puck-GG	Puck	10	6	ID23-1 ▾	3 ▾
ship-AR	03-09-2014	Dewar1	ESRF0306914	puck-22	Puck	10	12	ID23-1 ▾	2 ▾
WF-realXtals	24-03-2014	dewar1	ESRF0306413	AAA008A-Cristiano	Basket	10	10	ID29 ▾	1 ▾
WF-realXtals	24-03-2014	dewar1	ESRF0306413	CN085A-Emi2	Puck	10	10	ID29 ▾	▾
WF-realXtals	24-03-2014	dewar1	ESRF0306413	AA374A-step2	Puck	10	10	ID29 ▾	▾
WF-realXtals	24-03-2014	dewar1	ESRF0306413	CB340A-Step1	Puck	10	10	ID29 ▾	▾
WF-realXtals	24-03-2014	dewar1	ESRF0306413	CF042A-AZ	Puck	10	10	ID29 ▾	▾

What is ISPyB : Preparing BioSaxs experiment

EXPERIMENT PREPARATION

Macromolecule Definitions

Experiment Design

Experiment Set up

Volume Requirements

Logistics

Samples imported from SMIS or manually added

Apriori sample information: PDB, sequences, stoichiometry, etc...

Macromolecules

Acronym	EDIT
BSA	EDIT
Camodulin	EDIT
Camodulin+EGTA	EDIT
Lipase B	EDIT
Lipase B DTT	EDIT
Lipase B 1-0 M	EDIT
Lipase B 1-0 M D	EDIT
Lipase B 1-5 M	EDIT
Lipase B 1-5 M D	EDIT
Lipase B 2-0 M	EDIT

Buffers

Acronym	EDIT
Hepes	EDIT
Tris	EDIT
bufferName	EDIT
code	EDIT

Experiments

Name	Macromolecules	EDIT	REMOVE
1 Just another test	Lipase B, BSA	EDIT	REMOVE
2 melissa_test	d1, d2	EDIT	REMOVE
3 aaaProteins_ver1	aaaProteins, aProtein, aaProtein	EDIT	REMOVE
4 Test Slots	BSA	EDIT	REMOVE

BSA

General Assembly Advanced

Name: Bovine Serum Albumin
Long name. I.e. Bovine serum albumin

Acronym: BSA
Acronym will be used in the files and analysis. I.e. BSA

Mol. Mass (Da): 4
Atomic mass estimation measured in Da

Extinction coef.: 5 Symmetry: P1

Refractive Index: 1 Solvent Viscosity: 2
How radiation propagates through the medium

Comments:

Save Close

BSA

General Assembly Advanced

This is required information for rigid body modeling

Contact Description File: Upload

Go to [SASREF manual](#) for further information

Add Modeling Option (FDB)

PDB	Symmetry	Multiplicity	REMOVE
dimer.pdb	P1	1	REMOVE
monomer.pdb	P1	1	REMOVE

I want rigid body modeling run on this stuff

ISPyB files/data as input of some of the Online Data Analysis Tools

What is ISPyB : Preparing BioSaxs experiment

EXPERIMENT PREPARATION

- Macromolecule Definitions
- Experiment Design
- Experiment Set up
- Volume Requirements
- Logistics

BIOSAXS Experiment Designer

Define Measurements

Define only the macromolecule's measurement you want to make. This wizard will add **buffers' measurement needed for subtraction automatically.**

Concentration Series | Individual Measurement

Macromolecules: Lipase B DT Buffer: Hepes

How many unknown concentrations do you have?: 3

Exposure. Temp.: 4 Vol. To Load (µl): 40 Transmission (%): 100

Wait Time: 0 SC Viscosity: low Flow:

Add

Measurements

Specimen				Parameters						Comments	
Macromo.	Conc.	Buffer	Exp. Temp.	Vol. Load	Trans.	Wait T.	Flow	Viscosity			
■ BSA	1.000	■ Tris	4.00 c	40.00 µl	100 %	0 s	yes	low	REMOVE		
■ BSA	2.000	■ Tris	4.00 c	40.00 µl	100 %	0 s	yes	low	REMOVE		
■ BSA	3.000	■ Tris	4.00 c	40.00 µl	100 %	0 s	yes	low	REMOVE		
■ Lipase B DTT	1.000	■ Hepes	4.00 c	40.00 µl	100 %	0 s	yes	low	REMOVE		
■ Lipase B DTT	2.000	■ Hepes	4.00 c	40.00 µl	100 %	0 s	yes	low	REMOVE		
■ Lipase B DTT	3.000	■ Hepes	4.00 c	40.00 µl	100 %	0 s	yes	low	REMOVE		

Ready

Next

What is ISPyB : Preparing BioSaxs experiment

EXPERIMENT PREPARATION

- Macromolecule Definitions
- Experiment Design
- Experiment Set up
- Volume Requirements
- Logistics

Measurements
Specimens
Requirements

Deep Well

A	○	○	○	○	○	○	○	○	○	○	○	○
B	○	○	○	○	○	○	○	○	○	○	○	○
C	○	○	○	○	○	○	○	○	○	○	○	○
D	○	○	○	○	○	○	○	○	○	○	○	○
E	○	○	○	○	○	○	○	○	○	○	○	○
F	○	○	○	○	○	○	○	○	○	○	○	○
G	○	○	○	○	○	○	○	○	○	○	○	○
H	○	○	○	○	○	○	○	○	○	○	○	○
	1	2	3	4	5	6	7	8	9	10	11	12

4 x (8 + 3) Block

A	●	●	●	●	●	●	●	●	●	○	○	○
B	●	●	○	○	○	○	○	○	○	○	○	○
C	○	○	○	○	○	○	○	○	○	○	○	○
D	○	○	○	○	○	○	○	○	○	○	○	○

96 Well plate

A	○	○	○	○	○	○	○	○	○	○	○	○
B	○	○	○	○	○	○	○	○	○	○	○	○
C	○	○	○	○	○	○	○	○	○	○	○	○
D	○	○	○	○	○	○	○	○	○	○	○	○
E	○	○	○	○	○	○	○	○	○	○	○	○
F	○	○	○	○	○	○	○	○	○	○	○	○
G	○	○	○	○	○	○	○	○	○	○	○	○
H	○	○	○	○	○	○	○	○	○	○	○	○
	1	2	3	4	5	6	7	8	9	10	11	12

Plate Types ▾ | Auto Fill ▾ | Empty ▾ | Zoom In ▾

Macromolecule	Buffer	Conc. ▲	Vol. Well	Plate	Row	Well
Buffers						
	Tris		240.00 µl	1	A	10
	Hepes		560.00 µl	1	A	9
aProtein						
aProtein	Hepes	1.250 mg/ml	40.00 µl	1	A	4
aProtein	Hepes	10.000 mg/ml	40.00 µl	1	A	1
aProtein	Hepes	2.500 mg/ml	40.00 µl	1	A	3
aProtein	Hepes	5.000 mg/ml	40.00 µl	1	A	2
aaProtein						
aaProtein	Tris	1.000 mg/ml	40.00 µl	1	A	7
aaProtein	Tris	3.750 mg/ml	40.00 µl	1	A	6
aaProtein	Tris	7.500 mg/ml	40.00 µl	1	A	5
aaaProteins						
aaaProteins	Hepes	2.000 mg/ml	40.00 µl	1	B	2
aaaProteins	Hepes	3.000 mg/ml	40.00 µl	1	B	1
aaaProteins	Hepes	6.000 mg/ml	40.00 µl	1	A	8

What is ISPyB : Preparing BioSaxs experiment

EXPERIMENT PREPARATION

Macromolecule Definitions

Experiment Design

Experiment Set up

Volume Requirements

Logistics : Dewar tracking

Estimation of required Volume

Go to Shipment

Specimen	Estimated Volume	Stock Solution
Hepes	560.00 µl	NEW STOCK SOLUTION
Tris	240.00 µl	NEW STOCK SOLUTION
aProtein + Hepes	160.00 µl	NEW STOCK SOLUTION
aaProtein + Tris	120.00 µl	NEW STOCK SOLUTION
aaaProteins + Hepes	120.00 µl	NEW STOCK SOLUTION

Edit Case

Code: test OPENED
Sessions: Mar 12th 15
Comments:

Courier Accounts Details for Return

Track Number From Synchrotron: Transport Value:
Track Number To Synchrotron: Storage Location:

Stock Solutions

[Add Stock Solution](#) [Add Existing](#)

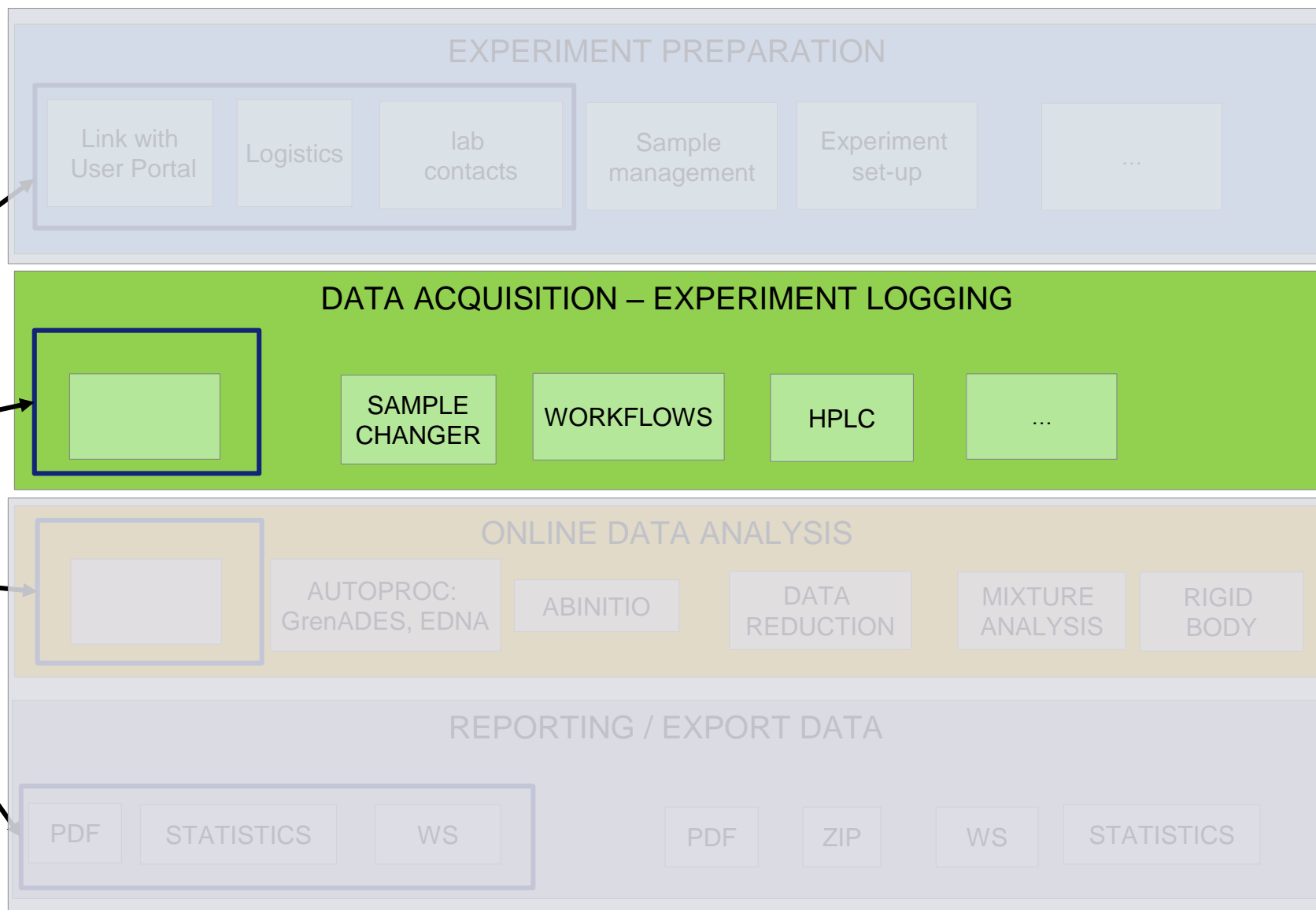
Macromolecule	Buffer	Storage Temp.	Volume	Concentration	Comments	
Amacr	Buffer	22.00 c	400.00 µl	12.00 mg/ml		EDIT UNPACK

Save Cancel

ISPyB Standard Dewar Tracking Protocol

ISPyB Features & Modules

Common to all techniques



What is ISPyB : EXPERIMENT LOGGING

Search DataCollection

Beamline: ID14-1 ID14-2 ID14-3 ID14-4 ID23-1
 ID23-2 ID29 ID30A-1 ID30A-2 ID30A-3
 ID30B BM14 BM16 BM29 BM30A
 ID19

Select all Beamlines Deselect all Beamlines

Start Date (DD/MM/YYYY): Start Time (hh:mm):

End Date (DD/MM/YYYY): End Time (hh:mm):

Search Reset

Last 11 DataCollections

Remove pagination

Beamline Name	Proposal	Image Prefix	Run No	# images	Status	Space Group	Completeness	Resolution	Rsymm Inner Outer Overall	Unit_cell a, b, c alpha, beta, gamma	Exp. Type	Protein Acronym	Start time	Skip	Cor
ID30A-3	OPID30a3	opid30a3	2	1							OSC		15:52:28 19-03-2015	<input type="checkbox"/>	
ID30A-3	OPID30a3	opid30a3	1	1							OSC		15:52:06 19-03-2015	<input type="checkbox"/>	
ID30A-3	OPID30a3	opid30a3	1	1							OSC		15:22:51 19-03-2015	<input type="checkbox"/>	
ID30A-3	OPID30a3	opid30a3	1	1							OSC		15:02:23 19-03-2015	<input type="checkbox"/>	
ID30A-3	OPID30a3	opid30a3	2	1							OSC		13:10:06 19-03-2015	<input type="checkbox"/>	
ID30A-3	OPID30a3	opid30a3	1	1							OSC		13:09:44 19-03-2015	<input type="checkbox"/>	
ID30A-1	MX1633	mesh-FluPo l-mRNA 05	1	30							Helical		12:12:39 19-03-2015	<input type="checkbox"/>	

What is ISPyB : MX experiment logging

Session										
Save Comments		View All DataCollection				Expand All Collapse All Clear Grouping				
Experiment Type	Acronym Sample name	Image Prefi	Run#	Parameters	Results	Image Thumbnail	Crystal snapshot	Graph	Second Graph	Comments
Start time: 12:57:16 16-05-2014 (1 Item)										
MXPressE	CER-samp A04	CER-sampA	1	<i>Nb tot images:</i> 3817 <i>Nb images:</i> 3817 <i>Exp. time:</i> 0.04 s <i>Phi range:</i> 0.10 ° <i>Flux:</i> 1.69E11 ph/sec <i>Detector resolution:</i> 2.... <i>Transmission:</i> 13.74 <i>Wavelength:</i> 0.976 Å <i>Total expo time:</i> 133.2...	MXPressE ● EDNA dp ● GrenADES fp ● GrenADES pp ● Space Group: P 41 21 2 Completeness:					
Start time: 12:45:21 16-05-2014 (1 Item)										
MXPressE	CER-samp A03	CER-sampA	1	<i>Nb tot images:</i> 1797 <i>Nb images:</i> 1797 <i>Exp. time:</i> 0.04 s <i>Phi range:</i> 0.05 ° <i>Flux:</i> 2.62E11 ph/sec <i>Detector resolution:</i> 2.... <i>Transmission:</i> 21.64 <i>Wavelength:</i> 0.976 Å <i>Total expo time:</i> 58.46 s	MXPressE ● EDNA dp ● GrenADES fp ● GrenADES pp ● Space Group: P 41 21 2 Completeness:					
Start time: 12:37:37 16-05-2014 (1 Item)										
MXPressE	CER-samp A02	CER-sampA	1	<i>Nb tot images:</i> 1437 <i>Nb images:</i> 1437 <i>Exp. time:</i> 0.04 s	MXPressE ● EDNA dp ● GrenADES fp ●					

What is ISPyB : Data acquisition for BioSaxs experiment

Name	Type	Macromolecules	Status	Download	Measurements	Averaged	Subtractions	Time	Experiment Type: ALL
Mar 12th 15									
1 evgsuno	HPLC	HPLC_M	FINISHED					20:11:52	00
2 evgsst	HPLC	Information not available	FINISHED					18:18:25	00
3 name	HPLC	Information not available	FINISHED					18:28:58	00
4 name	HPLC	Information not available	FINISHED					18:21:09	00
5 name	HPLC	Information not available	FINISHED					18:19:57	00
6 name	HPLC	Information not available	FINISHED					18:13:54	00
7 name	HPLC	Information not available	FINISHED					18:11:14	00
8 BSA	HPLC	HPLC_M	FINISHED					17:06:46	00
9 BSALys.xml	STATIC	bsa	FINISHED	Download	3 of 3	3 of 3	1 of 1	18:56:30	00
10 BSALys.xml	STATIC	LYS, bsa	FINISHED	Download	13 of 13	13 of 13	6 of 6	15:34:09	00
11 Water.xml	CALIBRATION	Water	FINISHED	Download	3 of 3	3 of 3	1 of 1	14:44:16	00
12 name	HPLC	HPLC_M	FINISHED					11:55:00	00
13 Lys-BSA.xml	STATIC	lysozyme, bsa	FINISHED	Download	36 of 36	36 of 36	8 of 8	10:23:44	00
14 water.xml	STATIC	Water	FINISHED	Download	3 of 3	3 of 3	1 of 1	09:37:23	00
15 water.xml	STATIC	Water	FINISHED	Download	3 of 3	3 of 3	1 of 1	09:37:17	00
16 water.xml	STATIC	Water	FINISHED	Download	3 of 3	3 of 3	1 of 1	09:38:00	00
17 water.xml	STATIC	Water	FINISHED	Download	3 of 3	3 of 3	1 of 1	09:09:44	00
Mar 11th 15									
18 scip_ly_bsa.xml	STATIC	LYS, LYS, bsa	FINISHED	Download	17 of 17	17 of 17	8 of 8	18:57:04	00
19 scip_ly_bsa.xml	STATIC	LYS, LYS, bsa	ABORTED	Download	0 of 17	0 of 17	0 of 0	18:50:37	00
20 scip.xml	STATIC	bsa	FINISHED	Download	13 of 13	13 of 13	6 of 6	15:07:53	00

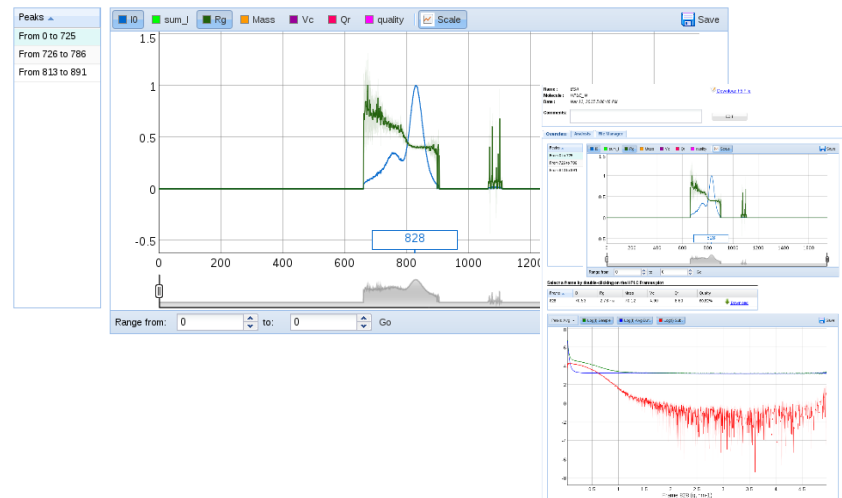
10	BSALys.xml	STATIC	LYS, bsa	FINISHED	Download	13 of 13	13 of 13	6 of 6	15:34:09	GO
11	Water.xml	CALIBRATION	Water	FINISHED	Download	3 of 3	3 of 3	1 of 1	14:44:16	GO
12	name	HPLC	HPLC_M	FINISHED					11:55:00	GO

SAMPLE CHANGER

Name: Lys-BSA.xml
 Type: STATIC
 Date: Mar 12, 2015 10:23:44 AM
 Comments: [BscCube] Generated from BscCube

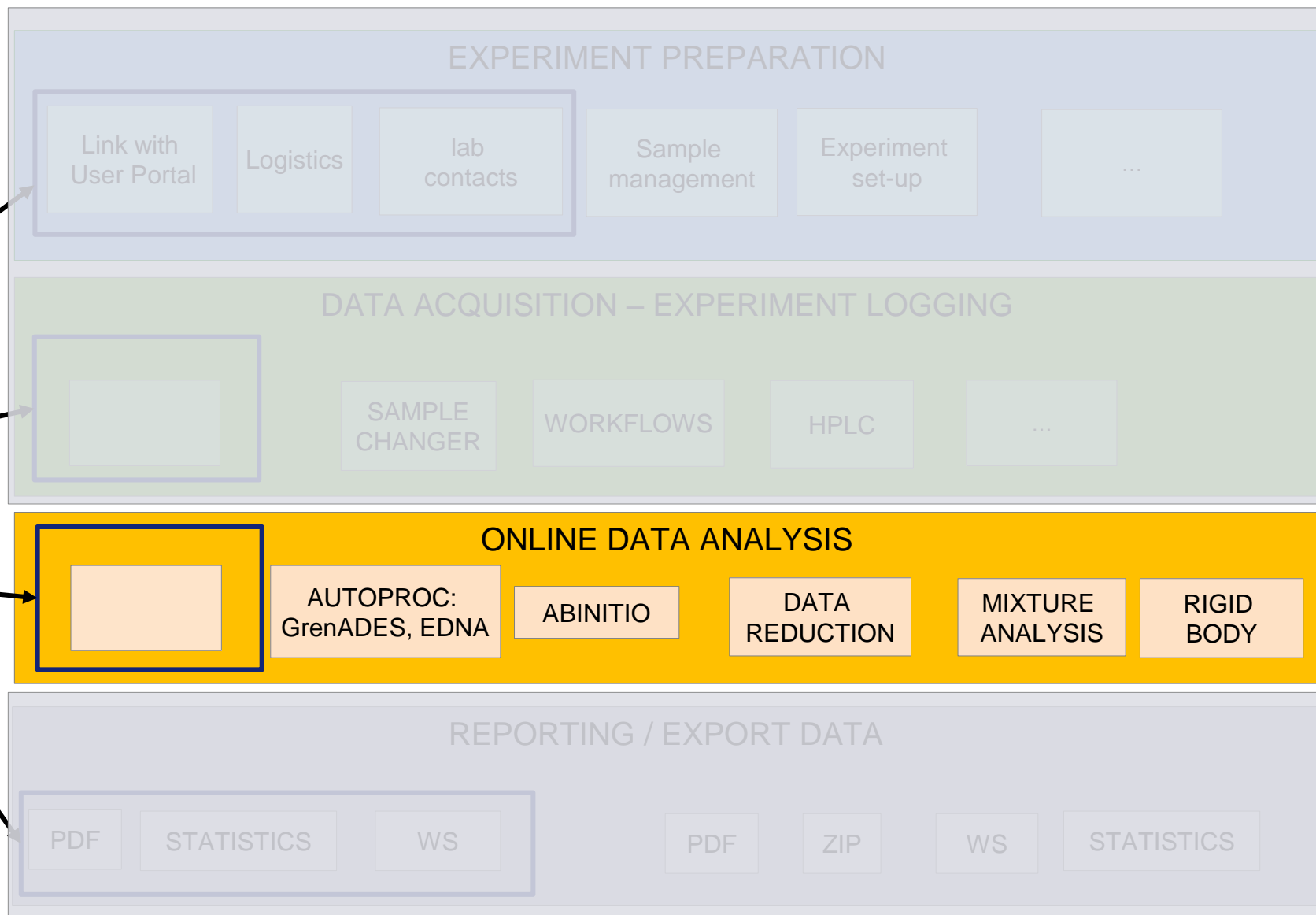
Macromolecule	Scattering	Frames (Averaged Total)	Q _{min}	Q _{max}	Quality	I(0)	Q ₀	Total	Draw	Volume	IMJ Vol. est.	AbRatio Modeling
lysozyme	1.00 mg/ml 20.00 °C	hepes (10 of 10) lysozyme (10 of 10) hepes (10 of 10)	1.47 nm	101 - 154 (53)	66.57 % ±2.5e-2	14.55	1.52 nm	0.80	5.13 ml	20.26 ml	10.1 - 13.5e	Download Primary Data Proc. AbRatio Modeling
lysozyme	5.00 mg/ml 20.00 °C	hepes (10 of 10) lysozyme (10 of 10) hepes (10 of 10)	1.53 nm	105 - 173 (68)	69.12 % ±2.4e-2	14.81	1.55 nm	0.80	5.35 ml	20.61 ml	10.3 - 13.7e	Download Primary Data Proc. AbRatio Modeling
lysozyme	2.00 mg/ml 20.00 °C	hepes (10 of 10) lysozyme (10 of 10) hepes (10 of 10)	1.54 nm	91 - 161 (110)	82.49 % ±1.4e-2	13.95	1.55 nm	0.79	5.39 ml	20.44 ml	10.2 - 13.6e	Download Primary Data Proc. AbRatio Modeling
bsa	3.00 mg/ml 20.00 °C	hepes (16 of 16) bsa (16 of 16) hepes (16 of 16)	3.10 nm	29 - 72 (43)	79.71 % ±4.6e-2	70.87	3.17 nm	0.61	10.84 ml	122.00 ml	61.0 - 81.3e	Download Primary Data Proc. AbRatio Modeling
bsa	1.70 mg/ml 20.00 °C	hepes (16 of 16) bsa (16 of 16) hepes (16 of 16)	3.28 nm	25 - 94 (29)	74.43 % ±7.7e-2	84.48	3.37 nm	0.56	11.81 ml	127.96 ml	64.0 - 85.3e	Download Primary Data Proc.

HPLC



ISPyB Features & Modules

Common to all techniques



What is ISPyB : MX experiment logging

Experiment parameters
Beamline parameters
AutoProcessing

Autoprocessing Summary (click on an entry for more details)

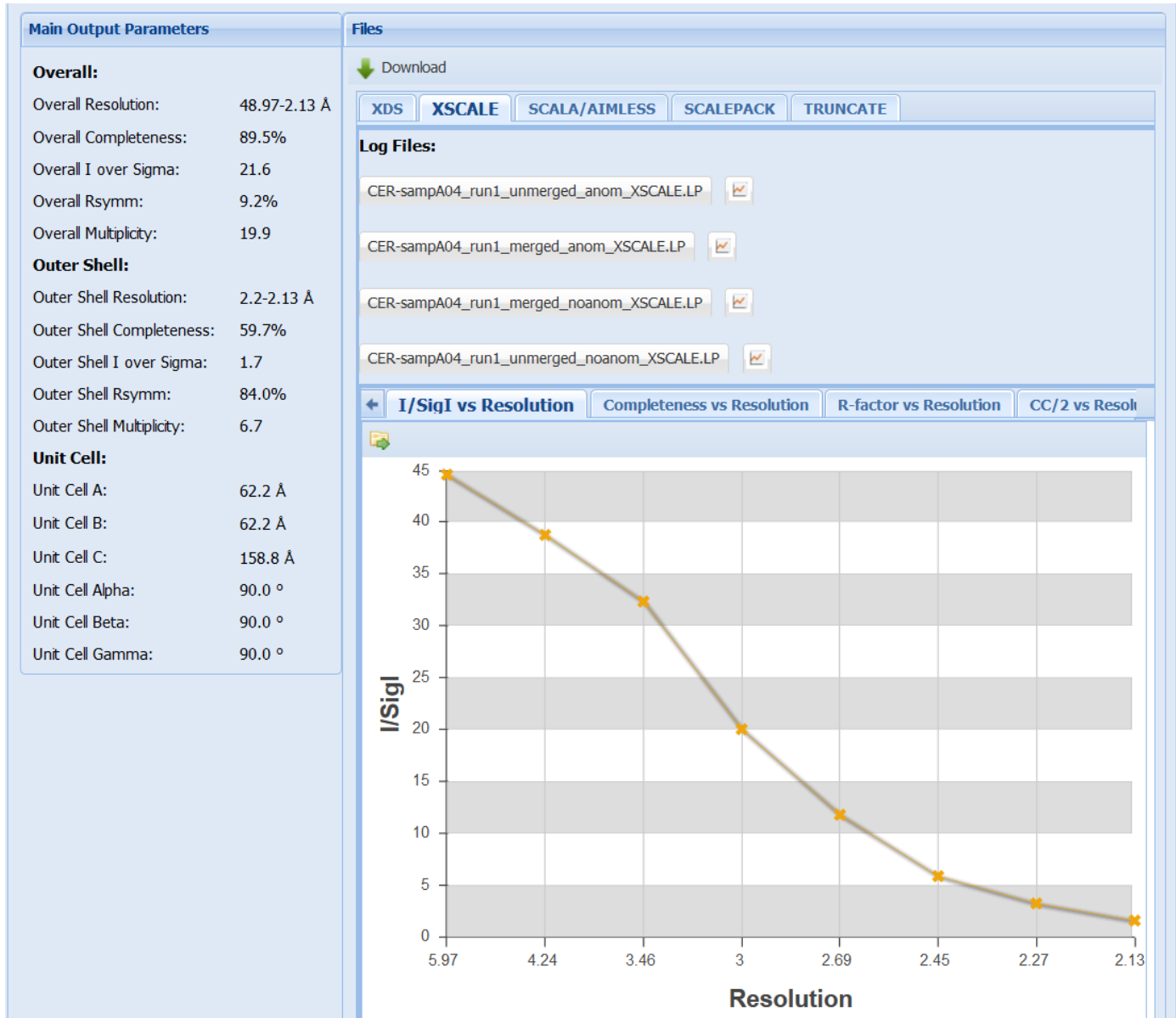
Method	Point Group	Cell A	Cell B	Cell C	Cell Alpha	Cell Beta	Cell Gamma
☑ Anomalous: OFF (Friedel pairs merged) (7 Items)							
EDNAproc	P 41 21 2	62.2	62.2	158.8	90	90	90
parallelproc	P 41 21 2	62.2	62.2	158.7	90	90	90
fastproc	P 4 2 2	62.2	62.2	158.7	90	90	90
parallelproc	P 4 2 2	62.2	62.2	158.7	90	90	90
parallelproc	P 4	62.2	62.2	158.7	90	90	90
parallelproc	C 2 2 2	87.9	88	158.7	90	90	90
parallelproc	P 1	62.2	62.2	158.8	89.9	90	90
☑ Anomalous: ON (Friedel pairs unmerged) (7 Items)							
parallelproc	P 41 21 2	62.2	62.2	158.7	90	90	90
EDNAproc	P 41 21 2	62.2	62.2	158.8	90	90	90
parallelproc	P 4 2 2	62.2	62.2	158.7	90	90	90
fastproc	P 4 2 2	62.2	62.2	158.7	90	90	90
parallelproc	P 4	62.2	62.2	158.7	90	90	90
parallelproc	C 2 2 2	87.9	88	158.7	90	90	90
parallelproc	P 1	62.2	62.2	158.8	89.9	90	90

RSymm threshold in lower shell:

I/Sigma threshold in lower shell:

View Data Collection Statistics:

What is ISPyB : MX experiment logging

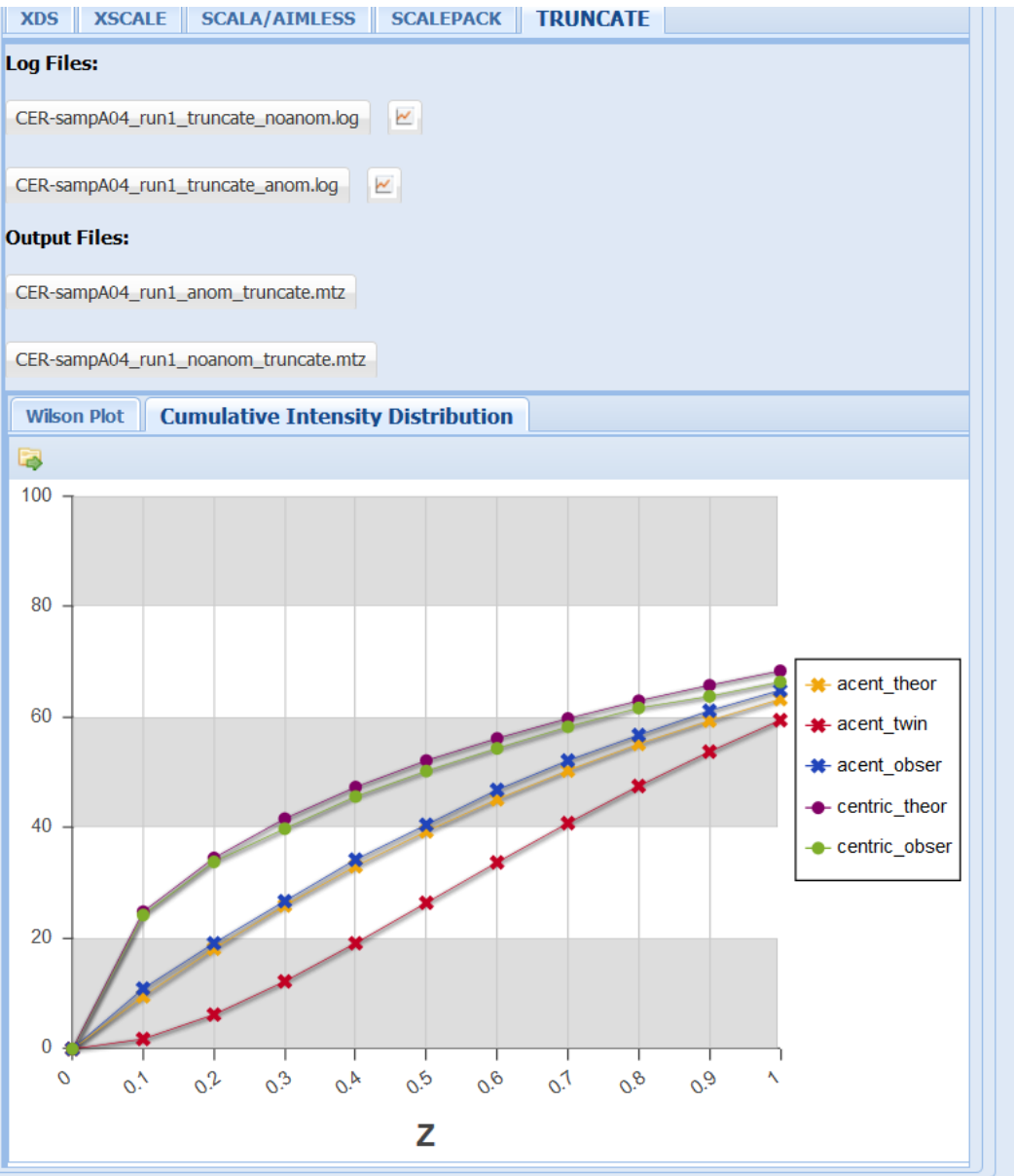


What is ISPyB : MX experiment logging

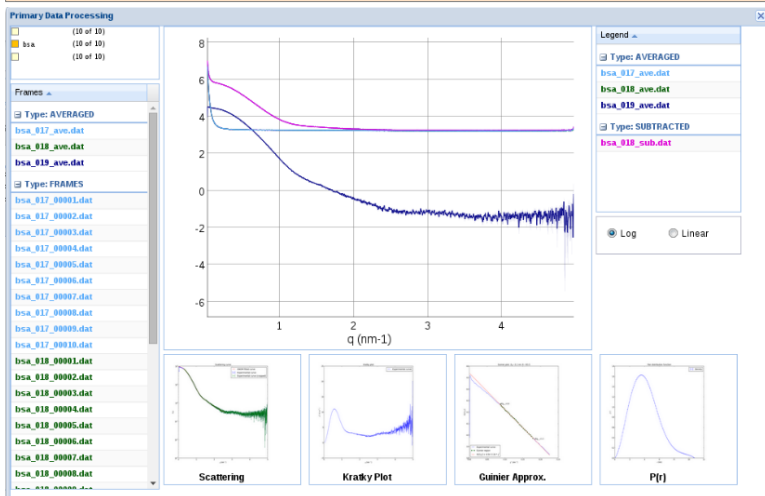
Overall Resolution: 48.97-2.13 Å
Overall Completeness: 89.5%
Overall I over Sigma: 21.6
Overall Rsymm: 9.2%
Overall Multiplicity: 19.9

Outer Shell:
Outer Shell Resolution: 2.2-2.13 Å
Outer Shell Completeness: 59.7%
Outer Shell I over Sigma: 1.7
Outer Shell Rsymm: 84.0%
Outer Shell Multiplicity: 6.7

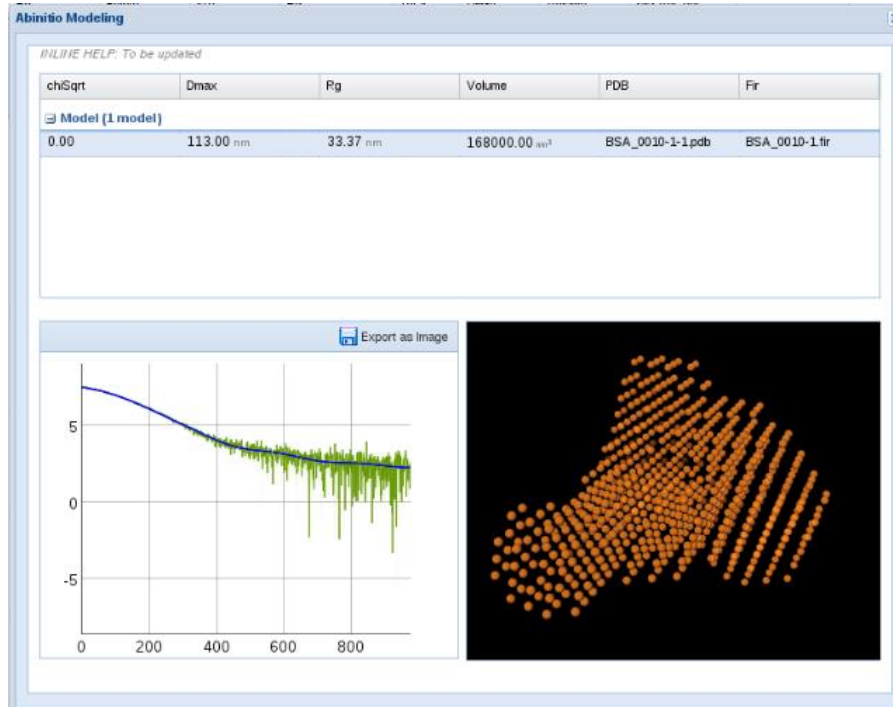
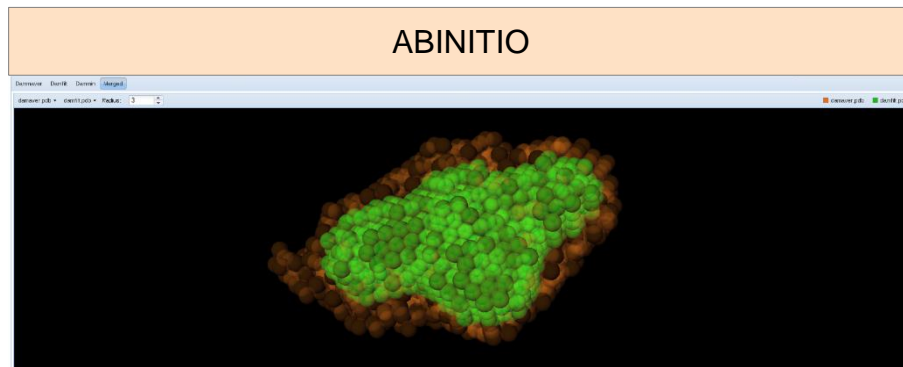
Unit Cell:
Unit Cell A: 62.2 Å
Unit Cell B: 62.2 Å
Unit Cell C: 158.8 Å
Unit Cell Alpha: 90.0 °
Unit Cell Beta: 90.0 °
Unit Cell Gamma: 90.0 °



DATA REDUCTION

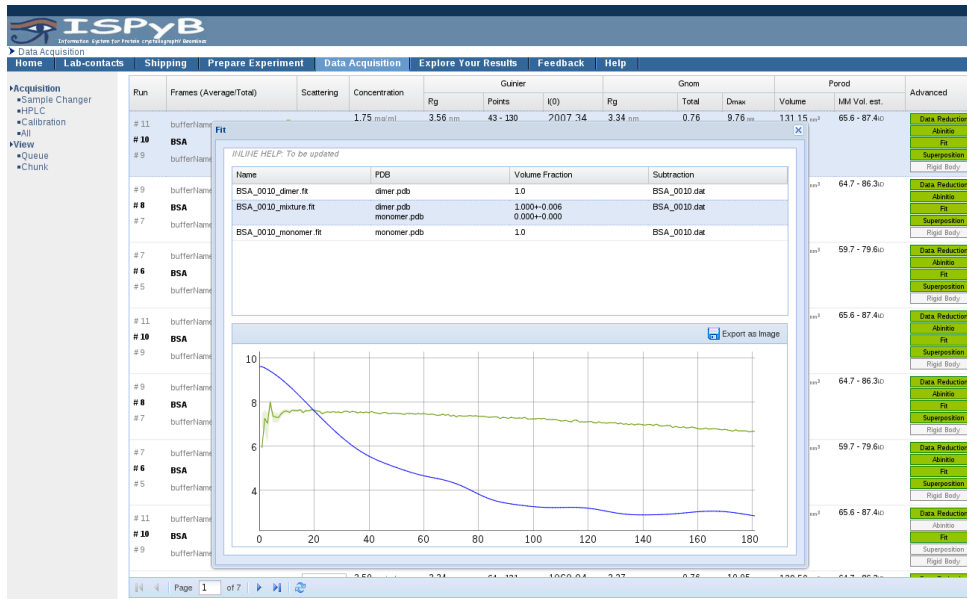


ABINITIO

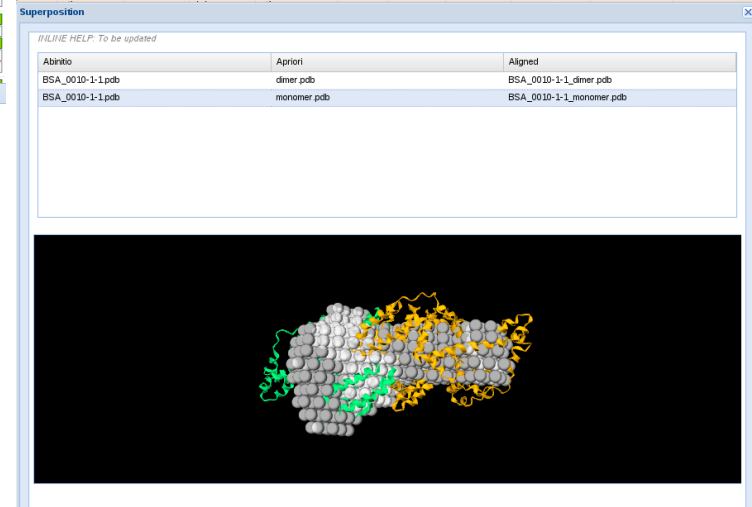


What is ISPyB : ONLINE DATA ANALYSIS

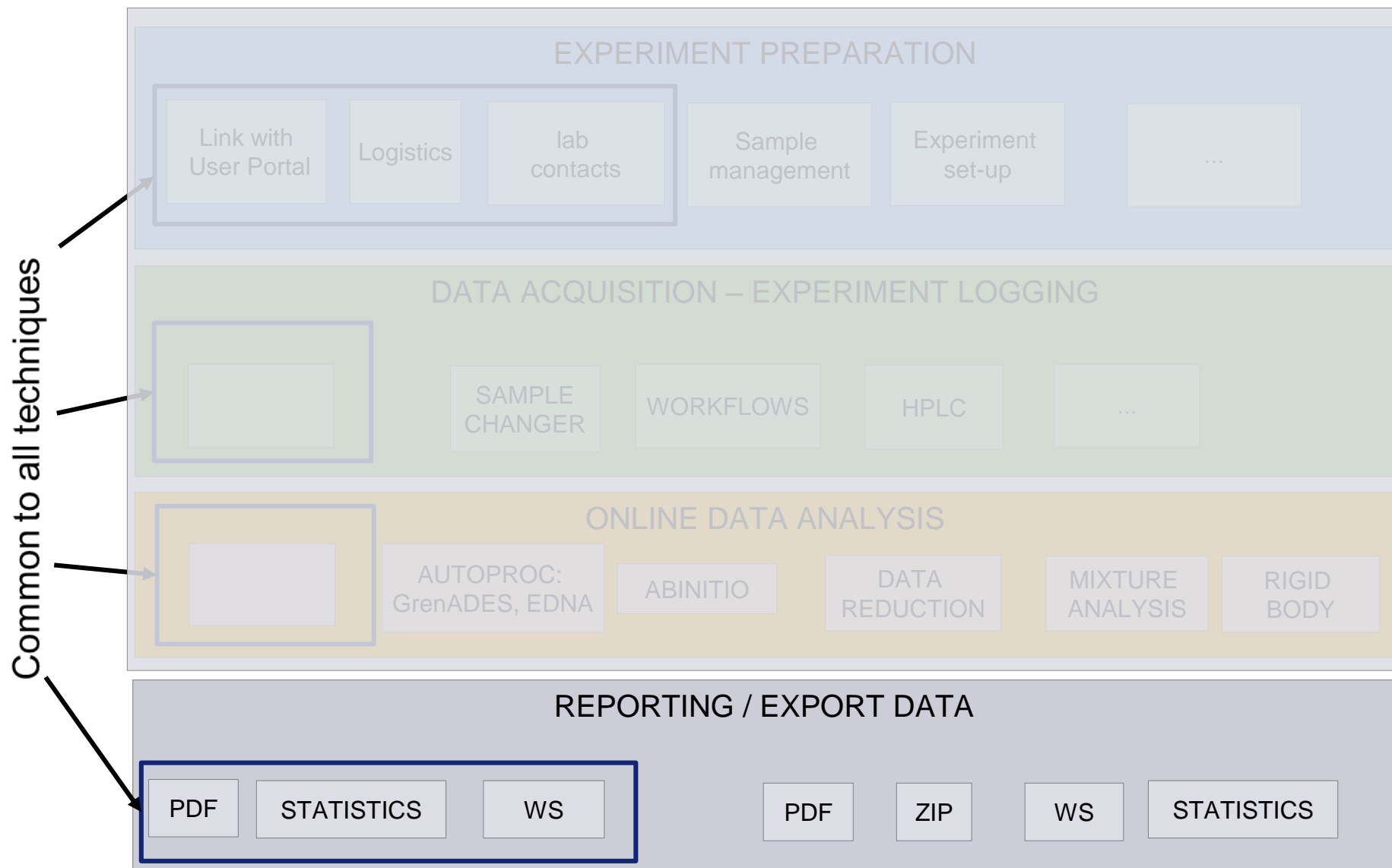
MIXTURE ANALYSIS



SUPERPOSITION



ISPyB Features & Modules



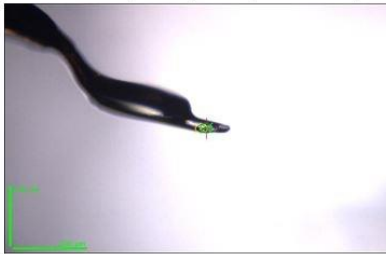
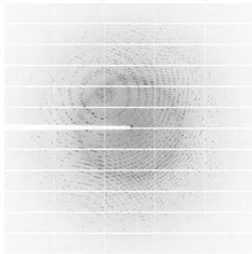
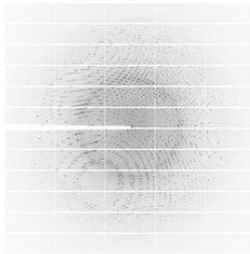
Long term tracking of experiments
 Process experiment results back into the Home LIMS
 Reports

Statistics on how e
 Screenings/Full data co
 Figures on feature usa

Data Collections for Proposal: opid291 on Beamline: ID29 --- Session start date: 04-10-2013

04/10/2013 12:04:58 Screen Image no 1: ice/powder ring detected. MOSFLM: Indexing successful (P3). Integrations successful. Strategy calculation successful.

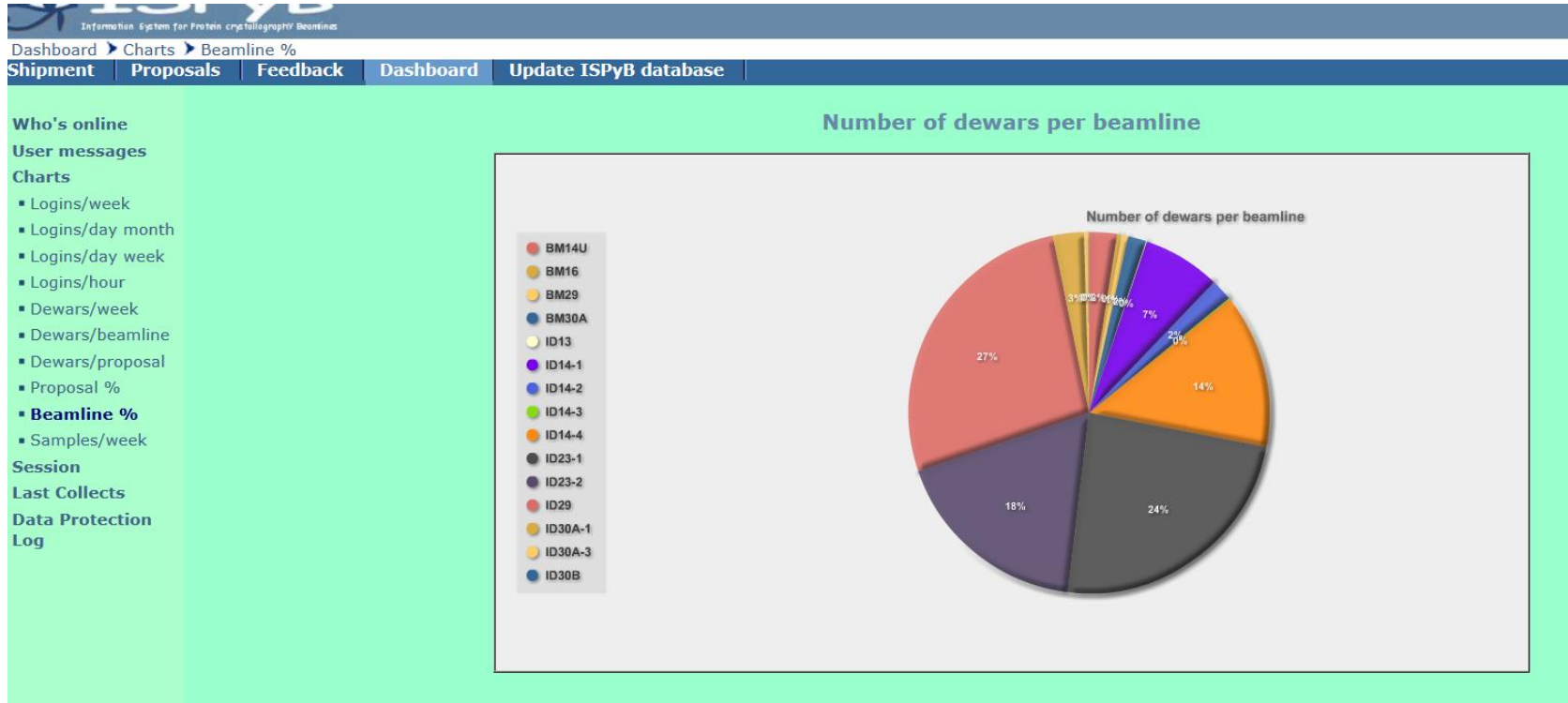
Image prefix	Run no	# images	Space Group	Unit Cell	Completeness (Inner, Outer, Overall)	Rsymm (Inner, Outer, Overall)	Resolution	Detector Resolution (Å)	Wavelength (Å)	Phi range (°)	Comments
ref-Thermolysin_xtal2	2	2						1.80	1.272	1.00	

Space Group	Unit Cell	Mosaicity (Å)	Ranking Resolution (Å)
P3	93.90 (90.00) 93.90 (90.00) 130.53 (120.00)	0.32	1.66

Wedge number	Resolution (Å)	Completeness	Multiplicity	Total dose	Number of Images	Phi (°)	Kappa (°)	Wavelength	Comments
1	1.7	100.0	4.4		548			1.3	

Sub Wedge number	Rotation axis	Axis start	Axis end	Exposure time	Transmission	Oscillation Range	Completeness	Multiplicity	Total dose	Number of images	Comments
1		87.0	224.0	0.1	16.4	0.2				548	



The structural biologist's best friend

Users on site or remote

Description of my shipment => Sample tracking

Description of my samples => Simplify my experiment

Real-time data analysis => Helps decision making during the experiment

Experiment reporting => experiment precise logbook

Data mining => History of a project, easy auto-processing files extraction



The beamline staff's best friend

Local contacts : Dewar tracking + monitoring of the collected data

Managers : Monitoring of the collected data + statistics

Stores : Dewar tracking, delivering, sending

Blom : Dewar tracking + statistics on a beamline

Java technology,

Struts (MVC Web Application Framework)

Hibernate (Object Relational Mapping)

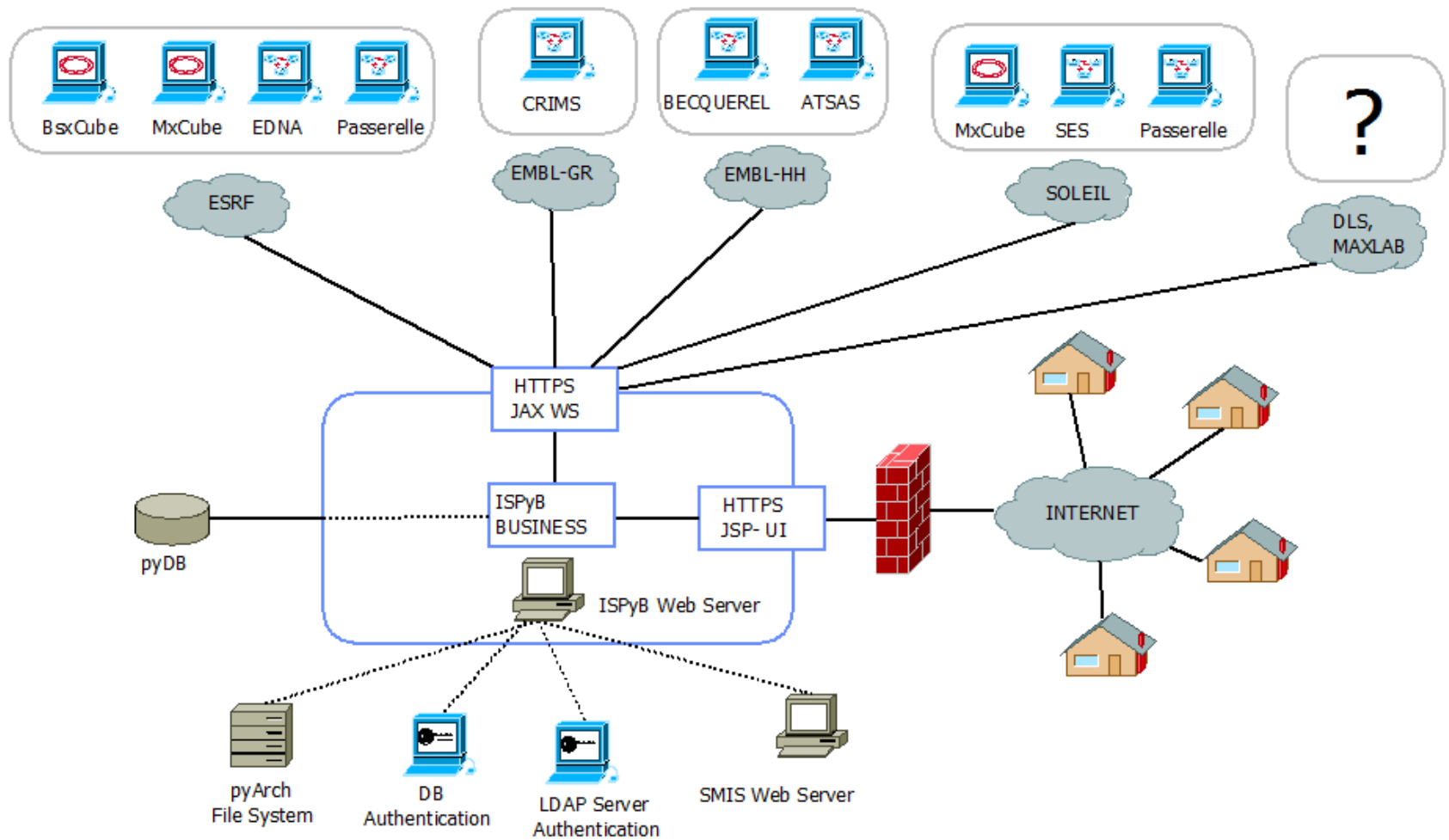
running on a JBoss 6 application server → WildFly 8.2 in June
supports both **MySQL** and **Oracle** databases (15-20 GB)

Sencha Ext JS 4: Javascript framework

Web services API (JAX-WS, SOAP)

Free software: **LGPL** licence





Common part

**Proposal
Shipment
Protein
Lab contact**

Macromolecules
Buffers
Assemblies
Additives

Data Acquisition
Sample Plates
Specimens
Measurements

+

Curve Analysis
Ab-initio Models

MX part

BioSAXS part

Roadmaps

Technical

Functional

Collaboration

Collaborations

Installed on several sites

1 to 1 : EMBLHH + EMBL Gre/ESRF thanks to Alejandro

1 to 1 : GA with Soleil

To formalize and materialize a pan-European collaboration

MOU, generic ISPyB ?

The screenshot shows the ISPyB web application interface. At the top, there is a search bar and the URL <http://forge.epn-campus.eu>. The navigation menu includes: Overview, Activity, Roadmap, Issues, New issue, Gantt, Calendar, News, Documents, Wiki, Files, Repository, and Settings. The main content area is titled "Overview" and contains the following information:

- Information System for Protein crystallographY Beamlines. ISPyB is a web based information management system for macromolecular (protein) crystallography X-ray experiments.
- Subprojects: BCR, ISPyB dev, ISPyBB, ISPyB WS Client
- Licence: LGPL

There is also an "Issue tracking" section with the following statistics:

- Bug: 42 open / 70
- Feature: 114 open / 131
- Support: 0 open / 0
- Action: 5 open / 8
- ToDo: 51 open / 59
- Maintenance: 0 open / 0

Links for "View all issues", "Calendar", and "Gantt" are provided. On the right side, there are sections for "Members" (listing Manager, Developer, and Reporter names) and "Latest news" (including "Repository has moved" and "Major release 3_0 now available").

Current ISPyB & ISPyBB version



- Last release of ISPyB is currently in test on following beamlines:
 - SWING for BioSAXS measurements
 - PROXIMA1 for MX measurements
 - PROXIMA2A for MX measurements

- Ongoing tasks or task to be done:
 - implementation of specific workflows for BioSAXS
 - new panels for HPLC measurements (in discussion with ESRF)
 - multi acquisition measurements (in discussion with ESRF)
 - connexion to MxCube
 - confidentiality regarding BAG proposals
 - sample tracking

Current ISPyB & ISPyBB version @ EMBL HH

Last release of ISPyB is currently in test on P12 (BioSaxs) from January 2015
→ **To be deployed in production on April 2015**

In test for MX

Current ISPyB & ISPyBB version @ MAX IV

Last release of ISPyB is currently in test

Thanks to

Alejandro De Maria Antolinos	EMBL/ESRF	Alun Ashton	DLS
Marjolaine Bodin	ESRF	Karl Levik	DLS
Emmanuel Eyer	ESRF	Darren Spruce	MAX IV
		Alberto Nardella	MAX IV
Stéphanie Malbet Monaco	ESRF	Marco Carmelenghi	EMBL HH
Elsbeth Gordon		Ivars Karpics	EMBL HH
Gordon Leonard	ESRF	Daniel Franke	EMBL HH
Sean Mc Sweeney		Dmitri Svergun	EMBL HH
Daniele De Sanctis	ESRF	Grégory Viguier	SOLEIL
Matthew Bowler	ESRF	Majid Ounsy	SOLEIL
Max Nanao	EMBL	Alain Buteau	SOLEIL
Adam Round	EMBL	Idrissou Chado	SOLEIL
Petra Pernot	EMBL	Angélique Prévost	SOLEIL
Martha Brennich	ESRF	Aurélien Thureau	SOLEIL
Andrew McCarthy	EMBL	Javier Perez	SOLEIL
		Pierre Legrand	SOLEIL
Olof Svensson	ESRF	Tatiana Isabet	SOLEIL
Matias Guijarro	ESRF	Andy Thompson	SOLEIL
Marcus Oscarsson	ESRF	Martin Savko	SOLEIL
Antonia Beteva	ESRF	William Shepard	SOLEIL
Thomas Boeglin	ESRF		
Jérôme Kieffer	ESRF		

...All the MX/BioSaxs beamline staff
...TID/MIS group
... people I forgot to mention (sorry)
... and all users for their constructive feedbacks

Do you have any questions about



?