What is ISPyB?

Solange Delagenière, MIS group, ESRF
What is ISPyB?

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:
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: BioStruct

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

- Proposal submission
- Online data analysis
- Reporting Data mining
- Experiment preparation
- Experiment
- Samples shipment
ISPyB Features & Modules

EXPERIMENT PREPARATION
- Link with User Portal
- Logistics
- Lab contacts
- Sample management
- Experiment set-up
- ...

DATA ACQUISITION – EXPERIMENT LOGGING
- SAMPLE CHANGER
- WORKFLOWS
- HPLC
- ...

ONLINE DATA ANALYSIS
- AUTOPROC: GrenADES, EDNA
- ABINITIO
- DATA REDUCTION
- MIXTURE ANALYSIS
- RIGID BODY

REPORTING / EXPORT DATA
- PDF
- STATISTICS
- WS
- PDF
- ZIP
- WS
- STATISTICS
What is ISPyB: let's log in

ICAT F2F meeting: What is ISPyB? | March 31st 2015 | Solange Delageniere
What is ISPyB: let’s log in

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

Login

Login

Password (*)

(*) 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).

Login  Reset

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.
Welcome

Select the proposal you want to work on:

<table>
<thead>
<tr>
<th>Proposals</th>
<th>Title</th>
<th>Type</th>
<th>GO</th>
</tr>
</thead>
<tbody>
<tr>
<td>☑️ SAXS</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MX415</td>
<td>TEST</td>
<td></td>
<td>GO</td>
</tr>
<tr>
<td>☑️ MX</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>IN905</td>
<td>Analysis of strain and Ge concentration on electronic substra...</td>
<td>MX</td>
<td>GO</td>
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<td>EDDAM project</td>
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<td>GO</td>
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<td>GO</td>
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<td>3D characterization of a catalytic membrane based on PLI an...</td>
<td>MX</td>
<td>GO</td>
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<tr>
<td>MX415</td>
<td>TEST</td>
<td>MX</td>
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</tr>
<tr>
<td>MX410</td>
<td>TEST PROPOSAL FOR CS-MIS GROUP</td>
<td>MX</td>
<td>GO</td>
</tr>
</tbody>
</table>
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: Any facility involved can make use of this feature to embed ISPyB inside their User Office web application.
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:
1. Define a shipment, containing stock solutions and cases
2. 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:
1. Create new samples for experiment; sample description will be based on the protein you have submitted through "samplesheets"
2. Define the buffers you plan to use for data collection
3. 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:
1. Retrieve information about a particular session
2. Retrieve information about a particular data collection
3. Retrieve information about a particular session
4. 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:
1. Find all data collections you did for a macromolecule and an estimate of their quality
2. Compare results from different collections and sessions

Currently your proposal contains:
0 Data Collections
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- WS
- STATISTICS
What is ISPyB: creating and filling in shipments

Upload from Excel, or csv

Create shipment

or fill on line
**What is ISPyB: creating/retrieving lab-contacts**

Max IV: created in DB

ESRF, EMBL, SOLEIL: retrieved from SMIS
Dewar location tracking

Communication between users / ESRF staff

Dewar description (beamline, local contact, user address)

Labels automatically filled in

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

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
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 Damatrix code on your samples pins.

<table>
<thead>
<tr>
<th>Shipment name</th>
<th>Shipment creation date</th>
<th>Dewar label</th>
<th>Dewar barcode</th>
<th>Container code</th>
<th>Container type</th>
<th>Container capacity</th>
<th># samples</th>
<th>Beaming Location</th>
<th>Location in Sample Changer</th>
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<tbody>
<tr>
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<td>14-11-2014</td>
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<td>MASSIFSAD</td>
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<td>ESRF0306914</td>
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<td>dewar1</td>
<td>ESRF0306413</td>
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<td>ESRF0306413</td>
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<td>Puck</td>
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<td>10</td>
<td>ID29</td>
<td></td>
</tr>
</tbody>
</table>

Save
What is ISPyB: Preparing BioSaxs experiment

- Samples imported from SMIS or manually added
- Apriori sample information: PDB, sequences, stoichiometry, etc...

ISPyB files/data as input of some of the Online Data Analysis Tools
What is ISPyB: Preparing BioSaxs experiment

### 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
- **Macromolecules:** Lipase B DTT
- **Buffer:** HEPES
- **How many unknown concentrations do you have?** 3
- **Exposure Temp.:** 4
- **Vol. To Load (μL):** 40
- **Trans. (%):** 100
- **Flow:**
- **SC Viscosity:** LOW

#### Individual Measurement

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Parameters</th>
<th>Comments</th>
</tr>
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<tbody>
<tr>
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</tr>
<tr>
<td>BSA 2.000</td>
<td></td>
<td>REMOVE</td>
</tr>
<tr>
<td>BSA 3.000</td>
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<td>REMOVE</td>
</tr>
<tr>
<td>Lipase B DTT 1.000</td>
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<td>REMOVE</td>
</tr>
<tr>
<td>Lipase B DTT 2.000</td>
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<tr>
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### Measurements

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</tr>
</thead>
<tbody>
<tr>
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<td>Tris</td>
<td>40.00 °C</td>
<td>40.00 μL</td>
<td>100 %</td>
<td>0 s</td>
<td>yes</td>
<td>low</td>
<td>REMOVE</td>
</tr>
<tr>
<td>BSA</td>
<td>2.000</td>
<td>Tris</td>
<td>40.00 °C</td>
<td>40.00 μL</td>
<td>100 %</td>
<td>0 s</td>
<td>yes</td>
<td>low</td>
<td>REMOVE</td>
</tr>
<tr>
<td>BSA</td>
<td>3.000</td>
<td>Tris</td>
<td>40.00 °C</td>
<td>40.00 μL</td>
<td>100 %</td>
<td>0 s</td>
<td>yes</td>
<td>low</td>
<td>REMOVE</td>
</tr>
<tr>
<td>Lipase</td>
<td>1.000</td>
<td>HEPES</td>
<td>40.00 °C</td>
<td>40.00 μL</td>
<td>100 %</td>
<td>0 s</td>
<td>yes</td>
<td>low</td>
<td>REMOVE</td>
</tr>
<tr>
<td>Lipase</td>
<td>2.000</td>
<td>HEPES</td>
<td>40.00 °C</td>
<td>40.00 μL</td>
<td>100 %</td>
<td>0 s</td>
<td>yes</td>
<td>low</td>
<td>REMOVE</td>
</tr>
<tr>
<td>Lipase</td>
<td>3.000</td>
<td>HEPES</td>
<td>40.00 °C</td>
<td>40.00 μL</td>
<td>100 %</td>
<td>0 s</td>
<td>yes</td>
<td>low</td>
<td>REMOVE</td>
</tr>
</tbody>
</table>

**Ready**
### What is ISPyB: Preparing BioSaxs experiment

#### Experiment Preparation

**Macromolecule Definitions**

**Experiment Design**

**Experiment Setup**

**Volume Requirements**

**Logistics**

#### Macromolecule Definitions

**Experiment Design**

**Experiment Setup**

**Volume Requirements**

**Logistics**

---

#### Macromolecule Definitions

<table>
<thead>
<tr>
<th>Macromolecule</th>
<th>Buffer</th>
<th>Conc</th>
<th>Vol. (µl)</th>
<th>Plate</th>
<th>Row</th>
<th>Well</th>
</tr>
</thead>
<tbody>
<tr>
<td>aProtein</td>
<td>Heps</td>
<td>1.250 mg/ml</td>
<td>40.00 µl</td>
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<td>A</td>
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<td>Heps</td>
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<td>A</td>
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<td>A</td>
<td>2</td>
</tr>
</tbody>
</table>

---

#### Experiment Design

**Volume Requirements**

**Logistics**

---

#### Experiment Setup

**Volume Requirements**

**Logistics**

---

#### Volume Requirements

**Logistics**

---

#### Logistics

---

#### What is ISPyB

**Preparation BioSaxs experiment**
What is ISPyB: Preparing BioSaxs experiment

**Volume Requirements**

<table>
<thead>
<tr>
<th>Macromolecule</th>
<th>Estimated Volume</th>
<th>Stock Solution</th>
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<tbody>
<tr>
<td>Hapes</td>
<td>560.00 µl</td>
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<tr>
<td>Tris</td>
<td>240.00 µl</td>
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</tr>
<tr>
<td>sProtein + Hapes</td>
<td>160.00 µl</td>
<td>NEW STOCK SOLUTION</td>
</tr>
<tr>
<td>sProtein + Tris</td>
<td>120.00 µl</td>
<td>NEW STOCK SOLUTION</td>
</tr>
<tr>
<td>sProtein + Hapes + Tris</td>
<td>120.00 µl</td>
<td>NEW STOCK SOLUTION</td>
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</tbody>
</table>

**Logistics: Dewar tracking**

**ISPyB Standard Dewar Tracking Protocol**
ISPyB Features & Modules

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What is ISPyB: EXPERIMENT LOGGING

Search DataCollection

- 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

<table>
<thead>
<tr>
<th>Beamline Name</th>
<th>Proposal</th>
<th>Image Prefix</th>
<th>Run No</th>
<th># Images</th>
<th>Status</th>
<th>Space Group</th>
<th>Completeness</th>
<th>Resolution</th>
<th>Rsymm</th>
<th>Unit_cell</th>
<th>Exp. Type</th>
<th>Protein Acronym</th>
<th>Start time</th>
<th>Skip</th>
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### What is ISPyB: MX experiment logging

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<tr>
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<td>CER-samp A04</td>
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<tr>
<td><strong>Corona</strong></td>
<td>CER-samp A04</td>
</tr>
<tr>
<td><strong>Corona</strong></td>
<td>CER-samp A04</td>
</tr>
</tbody>
</table>

**Parameters**

- Nb tot images: 3817
- Nb images: 3817
- Exp. time: 0.04 s
- Phi range: 0.10°
- Flux: 1.69E11 ph/sec
- Detector resolution: 2.5 Å
- Transmission: 10.74
- Wavelength: 0.976 Å
- Total exposure time: 133.2... s

**Results**

- MyPressE
- EDNA dp
- GrenADES fp
- GrenADES dp

**Space Group:** P 41 2 1 2

**Completeness:**

- MyPressE
- EDNA dp
- GrenADES fp
- GrenADES dp

**Space Group:** P 41 2 1 2

**Completeness:**

- MyPressE
- EDNA dp
- GrenADES fp
- GrenADES dp

**Space Group:** P 41 2 1 2

**Completeness:**

- MyPressE
- EDNA dp
- GrenADES fp
- GrenADES dp

**Space Group:** P 41 2 1 2

**Completeness:**
What is ISPyB: Data acquisition for BioSaxs experiment

SAMPLE CHANGER

HPLC

DATA ACQUISITION – EXPERIMENT LOGGING
ISPyB Features & Modules

EXPERIMENT PREPARATION
- Link with User Portal
- Logistics
- lab contacts
- Sample management
- Experiment set-up
- ...

DATA ACQUISITION – EXPERIMENT LOGGING
- SAMPLE CHANGER
- WORKFLOWS
- HPLC
- ...

ONLINE DATA ANALYSIS
- AUTOPROC: GrenADES, EDNA
- ABINITIO
- DATA REDUCTION
- MIXTURE ANALYSIS
- RIGID BODY

REPORTING / EXPORT DATA
- PDF
- STATISTICS
- WS
- PDF
- ZIP
- WS
- STATISTICS
### What is ISPyB: MX experiment logging

#### Autoprocessing Summary (click on an entry for more details)

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<th>Cell B</th>
<th>Cell C</th>
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#### View Data Collection Statistics:

- RSymm threshold in lower shell: [Input Field]
- I/Sigma threshold in lower shell: [Input Field]
- Update button
What is ISPyB: MX experiment logging

Main Output Parameters

Overall:
- 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°

Log Files:
- CER-samp04_run1_unmerged_anom_XSCALE.LP
- CER-samp04_run1_merged_anom_XSCALE.LP
- CER-samp04_run1_merged_noanom_XSCALE.LP
- CER-samp04_run1_unmerged_noanom_XSCALE.LP

Graphs:
- I/Sig1 vs Resolution
- Completeness vs Resolution
- R-factor vs Resolution
- CC/2 vs Resolution
### What is ISPyB: MX experiment logging

**Log Files:**
- CER-sampa04_run1_truncate_noanom.log
- CER-sampa04_run1_truncate_anom.log

**Output Files:**
- CER-sampa04_run1_anom_truncate.mtz
- CER-sampa04_run1_noanom_truncate.mtz

### XDS Log File Details

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**Cumulative Intensity Distribution**

The graph shows cumulative intensity distribution with different markers indicating theoretical and observed intensities.
What is ISPyB: ONLINE DATA ANALYSIS

DATA REDUCTION

ABINITIO

ONLINE DATA ANALYSIS
What is ISPyB: ONpine DATA ANALYSIS

MIXTURE ANALYSIS

SUPERPOSITION
ISPyB Features & Modules

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Common to all techniques
What is ISPyB: MX DATA MINING

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

Statistics on how experiments carry out
Screenings/Full data collection
Figures on feature usage
What is ISPyB: Statistics

Dashboard > Charts > Beamline %

Who’s online
User messages
Charts
- Logins/week
- Logins/day month
- Logins/day week
- Logins/hour
- Dewars/week
- Dewars/beamline
- Dewars/proposal
- Proposal %
- Beamline %
- Samples/week
Session
Last Collects
Data Protection Log

Number of dewars per beamline
What is ISPyB?

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
Where is ISPyB going?

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 ?
Current ISPyB & ISPyBB version

- Last release of ISPyB is currently in test on following beamlines:
  - SWING for BioSAXS measurements
  - PROXMA1 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
Where is ISPyB going?

**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
References and Acknowledgements

Thanks to

<table>
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<tr>
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<th>Institution</th>
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<tr>
<td>Alejandro De Maria Antolinos</td>
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<td>Marjolaine Bodin</td>
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...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 ISPyB?