




ISPyB: The structural biologist's experiment companion

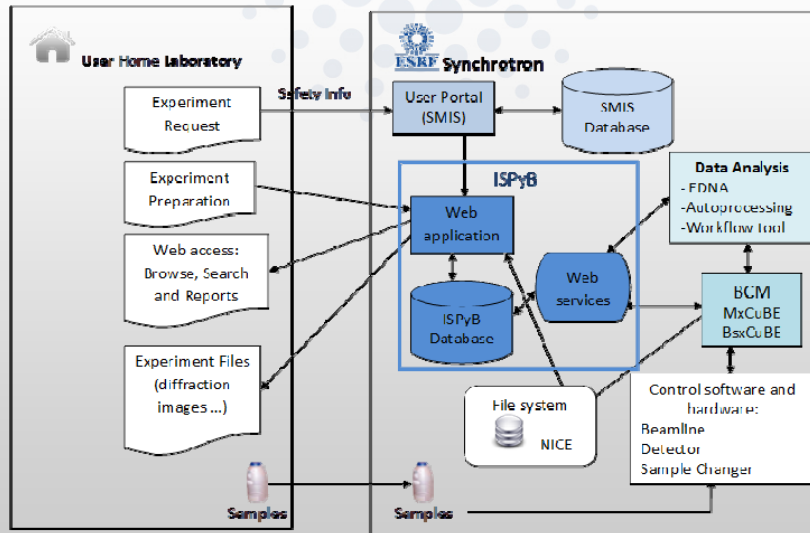
S. Monaco

- 
- What is ISPyB?
 - ISPyB : the structural biologist's experiment companion
 - Description of my shipment => Sample tracking
 - Description of my samples => Simplify my experiment
 - Real-time data storage => Helps decision making during the experiment
 - Experiment reporting => experiment precise logbook
 - Data mining => History of a project, easy autoprocesing files extraction
 - ISPyB “à la carte”
 - MX but also BIOSAXS companion
 - Conclusion & perspectives

- ISPYB is a Laboratory Information Management System (LIMS) linking **samples** to their corresponding **data**. It is a dynamic web application using a MySQL database.
- **Access to ISPYB?**
Through a web browser at <http://ispyb.esrf.fr>
To log-in: an ESRF Experiment number and password are required.
- **Why it has taken a more important role over the years** : to face the deluge of data coming from our detectors (i.e ~1900 data collections from MX beamlines in 2005, ~106500 in 2013)
- **History:**
 - 2001 - 2005: Pxweb (experiment reporting only)
 - 2005 - now: ISPYB (experiment reporting & much more)
 - joint development between the ESRF Joint Structural Biology Group (JSBG), BM14 (e-HTPX), the EU funded SPINE project
 - 2009: Collaboration with DLS (code sharing)
 - 2012: BioSAXS extension (collaboration between ESRF, EMBL HH & DLS [BioSTRUCT-X])



- Simplifying experiment preparation & execution
- Experiment reporting
 - The course of the experiment can be followed by colleagues in real time
- Real time experiment tracking & data analysis
 - Sample characterisation
 - Automatic data processing
 - Including download of processed data [h, k, l, I $\sigma(l)$ etc.]
 - Merged or unmerged



- Creating a 'shipment' in ISPyB allows the user to follow the shipment from and to his lab:
 - => automatic generation of labels (To and From ESRF) with a (unique) barcode

The image shows a screenshot of the ISPyB web interface on the left and a sample shipment label on the right.

ISPyB Web Interface: The 'Shipments' tab is highlighted. The page displays 'Welcome to User : mx415' and instructions for creating a shipment. A red circle highlights the 'Shipments' tab, and a red arrow points from it to the 'Shipments' section of the label.

Shipment Label: The label is addressed to 'ESRF Magasin, 6 rue Jules Horowitz, 38042 Grenoble, FRANCE'. It features a barcode at the top, a 'FRAGILE' warning, and a 'THIS WAY UP' arrow. The label includes fields for 'Prepared at', 'Prepared on', 'Experiment date', and 'Experiment name'. A red circle highlights the 'Prepared on' field, which contains the date '2014-02-13'.

- Creating a shipment in ISPyB allows the user to link it with an experimental session and:
 - => automatic population of labels with a barcode
 - => automatic emails upon arrival at stores & BLs to users, LC
 - => Follow-up of shipment history

The screenshot shows the ISPyB interface with the 'Dewar history view' open. The main table lists shipment events with columns for Date, Status, and Location. A sidebar on the left contains navigation options like 'Create', 'View', and 'Search'. A red circle highlights the 'Shipments' link in the sidebar, and another red circle highlights the 'History' link in the table's header.

Date	Status	Location
21-11-2012 16:31	ready to go	
22-11-2012 17:02	sent to ESRF	
23-11-2012 18:41	at ESRF	STONES-EM
23-11-2012 11:08	at ESRF	1070
23-11-2012 15:18	processing	
23-11-2012 15:38	processing	
23-11-2012 16:03	processing	
23-11-2012 16:04	processing	
04-12-2012 12:51	processing	
04-12-2012 12:01	ready to go	
05-12-2012 09:01	at ESRF	STONES-CHT
05-12-2012 14:09	sent to user	

- How to describe the samples in a shipment?
 - 3 ways : csv upload, Excel file upload, shipment description within ISPYB

The screenshot shows the ISPyB 'shipment' form. A table is used to describe the samples in the shipment. The table has columns for Sample, Position, Name, Pdbcode, Space, Group, Pre-Observed resolution, Needed resolution, Oscillation Range, Experiment, and several Unit Cell parameters. A red circle highlights the 'Sample' column header.

Sample	Position	Name (*)	Pdbcode	Space	Group	Pre-Observed resolution	Needed resolution	Oscillation Range	Experiment	Unit Cell a	Unit Cell b	Unit Cell c	Unit Cell alpha	Unit Cell beta	Unit Cell gamma	Comments
1	A-TM - P21212	samp01		P21212		0.0	0.0	0.0	OSC	0.0	0.0	0.0	0.0	0.0	0.0	
2	A-TM - P21212	samp02		P21212		0.0	0.0	0.0	OSC	0.0	0.0	0.0	0.0	0.0	0.0	
3	AS - Undefined	test01		Undefined		0.0			OSC							
4	A - P21212	crystal01		P21212		0	0	0	OSC	0	0	0	0	0	0	
5									OSC							
6									OSC							
7									OSC							



The screenshot displays the SB companion software interface. At the top, there's a menu bar with 'File', 'Instrumentation', and 'Help'. Below it, a 'Collect' button is visible. The main area is divided into several panels:

- Left Panel:** A list of sample positions from 1.1 to 2.9, with '1.3' selected.
- Top Center:** 'Sample centring' and 'Sample position' controls, including Omega (1241.4), Kappa (0.0), Phi (0.0), and sample length (23.71).
- Center:** A video feed showing the synchrotron beamline with a green box indicating the aperture. Below it are 'Aperture' controls (10, 20, 30, 50 micrometers) and 'Outbeam'.
- Right Panel:** 'Collection method' settings, including 'Discrete', 'Characterise', 'Medical', and 'Lines'. It also shows 'Acquisition' parameters like 'Oscillation range', 'Oscillation overlap', 'Exposure time', 'Energy (keV)', 'Resolution (Å)', and 'Transmission (%)'. There are also 'Data location' and 'Processing' options.
- Far Right:** A 'Machine current' panel showing 'Energy' (12.660 keV), 'Current' (12.660 A), and 'Move to' options.

 At the bottom, there are status messages: 'Measured values for background and X-ray intensity not very distinguishable.', 'Integrated counts for image : 143.771', and 'You have opened control of the application.'



- Characterisation of diffraction quality
 - EDNA, BEST

The screenshot shows the 'Characterisation Results' window. It contains two main sections:

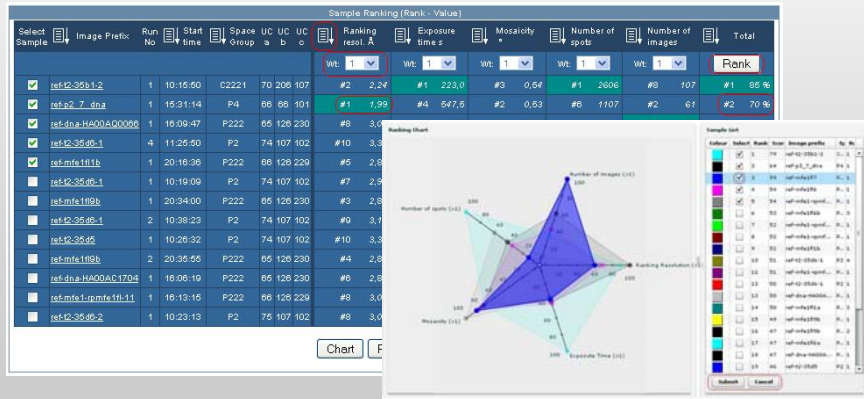
- Characterisation Results (EDNA log file):**
 - Data collection info:**

Data collection date	2012-Nov-23 14:05:24.666
Image prefix	refE09_1
Directory	data/629/inhouse/sg4291/20121123-RAW_DATA/zenifer/E09
 - Diffraction Plan:**

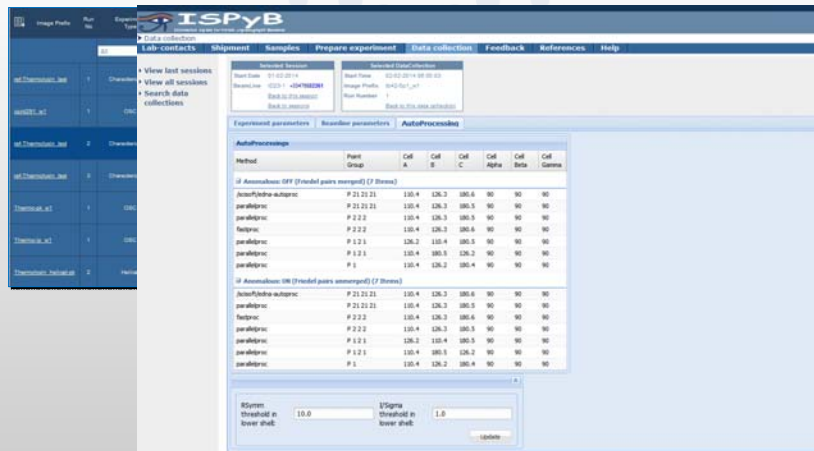
Forced space group	Anomalous data	Aimed multiplicity	Aimed completeness	Aimed images at highest res.	Aimed resolution (Å)
None	False	Default (optimized)	Default (= 0.99)	3.00	Default (highest possible)
- Collection plan strategy (RADDOSSE log file, BEST log file):**
 - Resolution limit is set by the radiation damage.

Wavelength (Å)	Start (°)	Width (°)	No. images	Exp. time (s)	Max res. (Å)	Std. dev. (%)	Distance (mm)
1	1	28.00	6.10	590	0.04	1.80	6.64
							351.02

- Sample ranking tool
 - Which are the best samples (*a priori*)?
 - Different metrics
 - Which are the best samples (*post data collection*)?



- Results of automatic data processing



The screenshot displays the SB companion software interface. It is divided into several sections:

- Experiment Parameters:** Includes tabs for 'Experiment parameters', 'Baseline parameters', and 'AutoProcessing'. It shows a table of 'AutoProcessing' results with columns for Method, Point Group, Cell A, Cell B, and Cell C. Below this are 'Main Output Parameters' and 'Files' sections.
- Main Output Parameters:** Lists overall statistics: Overall Resolution: 100.0-2.17 Å, Overall Completeness: 97.9%, Overall I over Sigma: 13.89, Overall Raymrs: 7.7%, Overall Multiplicity: 4.2. It also lists 'Outer Shell' parameters and 'Unit Cell' dimensions (A: 110.4 Å, B: 126.3 Å, C: 180.5 Å).
- Files:** Shows input and output files, including 'scale_noanom.inp', 'merged_noanom.sca.gz', and 'merged_noanom_XSCALE.LP'.
- Graphs:** A line graph titled 'I/SigI vs Resolution' plots I/SigI (y-axis, 0 to 36) against Resolution (x-axis, 4.67 to 2.17 Å). The data points show a decreasing trend as resolution increases.

The screenshot displays the SB companion software interface for experiment reporting. It features several key components:

- Parameters & Results:** A detailed view of experiment parameters and results, including 'Key Statistics' and 'Experiment Parameters'.
- Crystal Snapshots:** A grid of four images showing the crystal during the experiment.
- Image thumbnails:** A set of image thumbnails representing different stages or views of the experiment.
- XRF Spectrum:** A plot of 'Counts' versus 'Energy' showing a sharp peak at approximately 8.9 keV, with 'Spectrum' and 'Background' lines overlaid.
- Autoprocessing results:** A graph showing the results of the autoprocessing step, likely related to the resolution vs I/SigI data.
- Absorption Edge Scan:** A plot showing the absorption edge scan results, with multiple curves representing different samples or conditions.
- Reports:** A section titled 'Reports' with buttons for 'View DOC report', 'View PDF report', 'View HTML report', 'DOC Summary', and 'PDF Summary'.

Reports on all sessions, on the screenings, per sample :

- Searches at various levels => keep history of a project

Samples

Protein acronym

Data collections

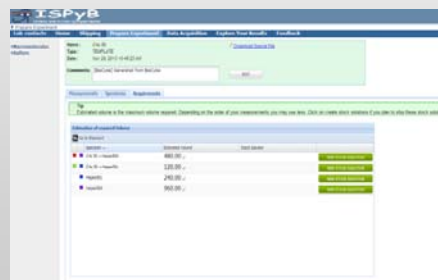
Image Profile	Run No.	Experiment Type	Protein Acronym	Start Time	# Images	Experiment Parameters Search	Status	Sample	Completeness	Resolution	Frames	Unit Cell	Space Group	Sample Handling	Ship	Comments	Download Automation File
	01																
	02																
	03																
	04																
	05																
	06																
	07																
	08																
	09																
	10																

- **1st level:** no action by the user.
Log on the beamline control software with experiment number: all parameters of that session will be stored in ISPYB – updated electronic logbook accessible from anywhere in the world
- **2nd level:** use of shipment description without pin barcodes
Same as in level 1. + experiment facilitated at the beamline (sample list in MxCuBE) + link crystal description and X-ray data
- **3rd level:** use of shipment description with pin barcodes
Same as 2nd level + allows user to make sure samples are placed correctly in the sample changer (mandatory to use MASSIF ?)

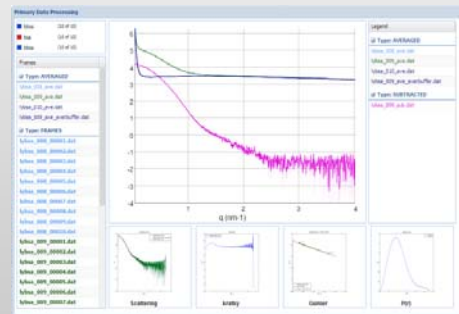
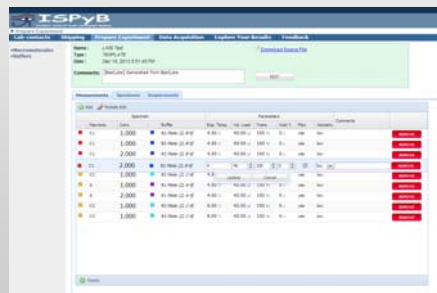
- Since 2012, same logging as for MX



- Since 2012, same logging as for MX
- **Experiment preparation** : input of sample information and the experimental aims provides feedback on the number of measurements required, calculation of expected sample volumes and time needed to collect the data



- Shipment tracking
- Online feedback, downstream analysis results, comparison of the results from new measurements with previous acquisitions to help guide the experiment
- *Ab initio* modeling results



primary data processing

- ISPyB: The structural biologist's experiment **unavoidable companion**.
 - Sample tracking to or from the synchrotron
 - **Electronic logbook** for MX and BIOSAXS experiments **assisting users** during their experiment (sample list, results view) but also **the memory** of a project
- In use at **several synchrotrons**:
 - DLS (MX)
 - DLS, Petra III, SOLEIL
- Main Perspectives:
 - MX : Storage of more **downstream data analysis results**
 - Results of (prototype) MR pipelines (Dimple)
 - Get **data collection plan** reworked to direct MASSIF beamlines tasks by sample diffraction plan precise definition
 - Continue Improving interfaces & tools
 - Currently each site has own DB. What about a fully European ISPyB?

Thanks to

The ISPyB team:

Marjolaine Bodin, Alejandro De Maria Antolinos,
Solange Delageniere, Elspeth Gordon, Stéphanie Monaco

Scientists involved (from EMBL-Grenoble & ESRF):

Matthew Bowler, Martha Brennich, Daniele De Sanctis, Gordon Leonard, Sean Mc Sweeney, Max Nanao, Petra Pernot, Adam Round

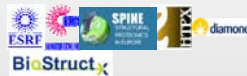
Former Staff

ESRF: Patrice Brenchereau, Ricardo Leal, Darren Spruce, Stéphanie Veyrier
BM14: Ludovic Launer, Martin Walsh

On site collaboration with other projects

MIS Group
EDNA, Workflow: Olof Svensson
EDNA for BioSAXS: Jérôme Kieffer
MXCuBE, BsxCuBE: Antonia Beteva, Matias Guijarro, Marcus Oscarsson
Auto processing: Thomas Boeglin

Collaboration with other synchrotrons
Diamond: Alun Ashton, Karl Levik
Petra IV: Dmitri Svergun



And

Thanks to all the users who take the time to send feedback and help us improve the software!