

# BAG training of 22/11/2005

## Demo 3 : ISPyB

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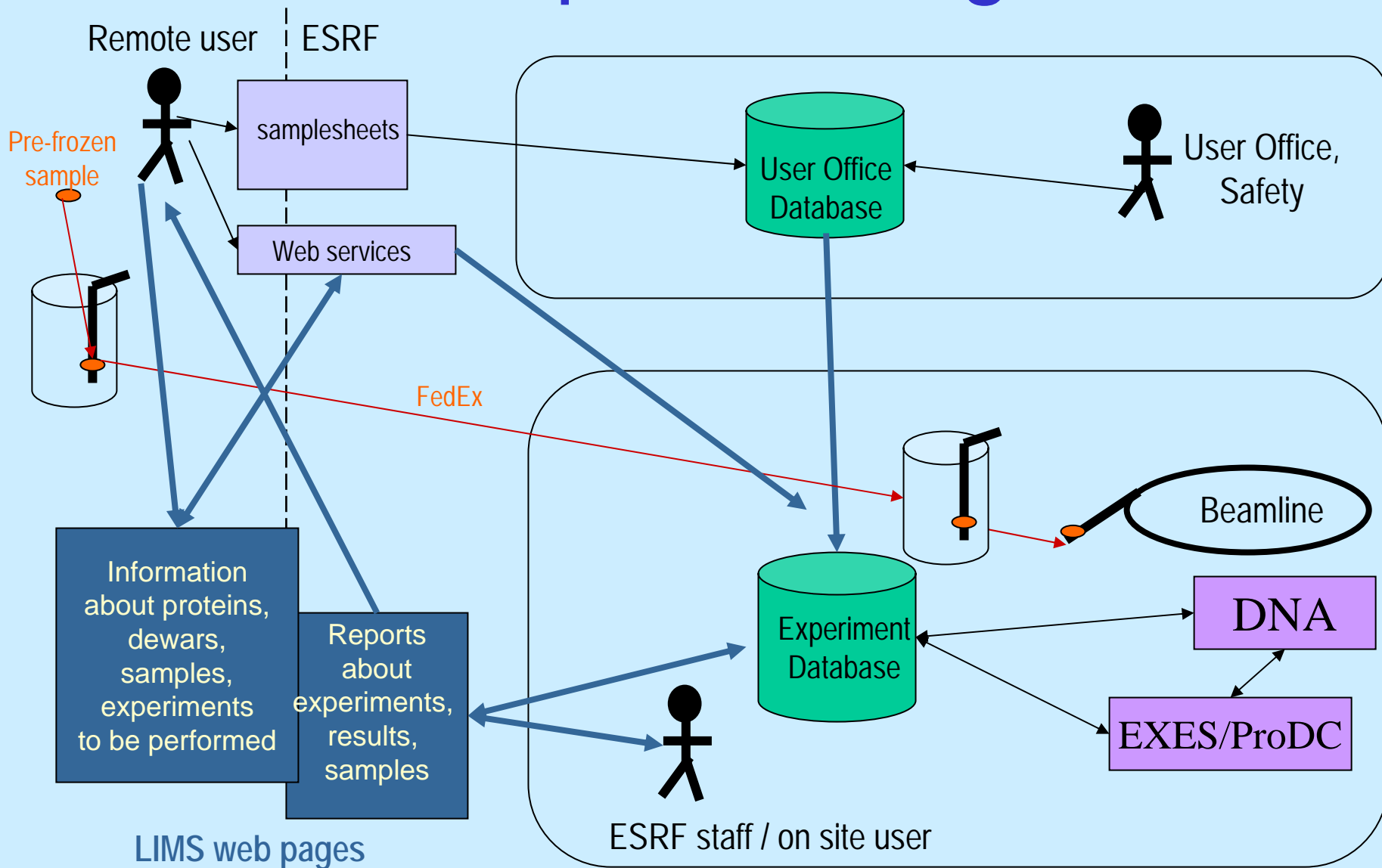
# Introduction

- Former PXWEB
  - Dedicated to ESRF: talking to DNA, ProDC, SMIS, User Office
  - Cope with the industrial requests: remote service
  - Compatible with sample changer : pipeline mode
- New ISPyB (Information System for Protein crystallographY Beamlines)
  - Joint development: ESRF, SPINE, eHTPX
  - Collaborations: EBI, BioXHit, DNA, ESRF information system group
  - Integrates all PXWEB features
  - Compatible with others projects (BAG submissions and reports), maintenance inside ESRF
  - Using Web services

# What is ISPyB ?

- ISPyB database
  - All data and parameters linked to the samples, shipments, data collections are stored
- ISPyB web application
  - Electronic log book
  - Remote or on-site access to the database

# Sample tracking



# ISPyB demo

## 1) From outside laboratory : preparing shipments

- 1) Retrieve new sample sheets
- 2) Create new crystal form
- 3) Create a shipment with samples

## 2) From ESRF:

- 1) Select a shipment for processing
- 2) Log-in to the Data collection GUI
- 3) Access samples prepared for experiment

## 3) View data collection and results

## 4) Search through old data

# ISPyB demo

## 1) From outside laboratory : preparing shipments

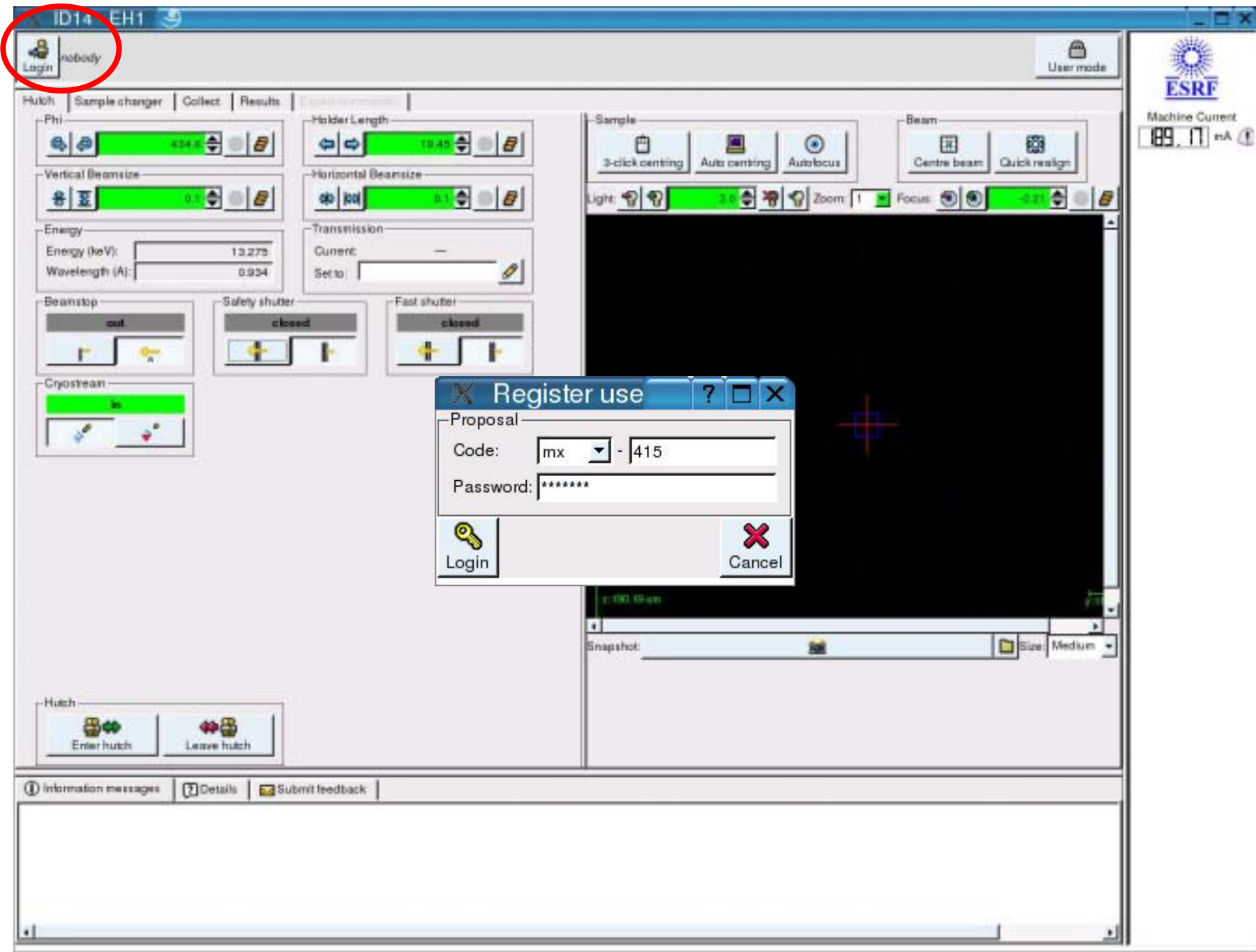
- 1) Retrieve new sample sheets
- 2) Create new crystal form
- 3) Create a shipment with samples

## 2) From ESRF:

- 1) Select a shipment for processing
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ID14 EH1

Login nobody

User mode



Machine Current  
189.17 mA

Hutch | Sample changer | Collect | Results

Phi: 434.5

Holder Length: 18.45

Vertical Beamsize: 0.1

Horizontal Beamsize: 0.1

Energy: 13.275 keV, 0.934 Å

Transmission: Current: --, Set to:

Beamstop: out

Safety shutter: closed

Fast shutter: closed

Cryostream: in

Sample: 3-click centring, Auto centring, Autofocus

Beam: Centre beam, Quick realign

Light: 3.0, Zoom: 1, Focus: -3.21

Register use dialog box with fields for Proposal Code (mx - 415) and Password (\*\*\*\*\*), and Login/Cancel buttons.

Hutch: Enter hutch, Leave hutch

Information messages | Details | Submit feedback

Window title: ID14 - ESRF

Logout **mx-415 TEST** MOCARTHY E.S.R.F. Dates: 2005-11-18 to 2005-11-18 User mode

Machine Current: **89.05** mA

**Beamline Parameters:**

- Phi: **-434.8**
- Holder Length: **10.45**
- Vertical Beamsize: **0.1**
- Horizontal Beamsize: **0.1**
- Energy (keV): **13.275**
- Wavelength (Å): **0.934**
- Transmission: **---**
- Current: **---**
- Set to:

**Shutters:**

- Beamstop: **out**
- Safety shutter: **closed**
- Fast shutter: **closed**

**Beamline Status:**

- Cryostream: **in**
- Hutch: **Enter hutch** / **Leave hutch**

**Sample & Beam Controls:**

- 3-click centring
- Auto centring
- Autofocus
- Centre beam
- Quick realign
- Light: **3.0**
- Zoom: **1**
- Focus: **-0.21**

**Image Display:**

- Snapshot:
- Size: **Medium**

**Footer:**

- Information messages
- Details
- Submit feedback

Select shipment - Mozilla

File Edit View Go Bookmarks Tools Window Help

http://ispyb.esrf.fr:8080/ispyb/user/prepareExp.do?reqCode=selectShipment

Home Bookmarks The Mozilla Cr... SuSE - The Lin... Logoff

# ISPyB

Prepare experiment > prepareExp.do

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

- Select a shipment
- Fill sample changer

First, select the shipments you want for processing. Then you will have to **fill the sample changer** assign a location in the sample changer to your containers

This second step is useless if you are using Datamatrix code on your samples pins.

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

Name	Shipping date	Courier name	Tracking number	Shipment status	Select for experiment	Save
pipeforNov05				processing	<input checked="" type="checkbox"/>	Save
slides plate	2005-10-19	tdt		opened	<input type="checkbox"/>	Save
sm14narcosFile	2005-10-21	DHL		opened	<input type="checkbox"/>	Save
scrt10	2005-10-19	fedex	22147	opened	<input type="checkbox"/>	Save
sm14	2005-10-14	JHL		processing	<input checked="" type="checkbox"/>	Save
1023-Test	2005-10-13	ESRF		closed	<input type="checkbox"/>	Save
scrt1005	2005-10-12	fedex	15667	closed	<input type="checkbox"/>	Save
2005-02-24E & PLF	2005-02-24	FedEx	7910382030	opened	<input type="checkbox"/>	Save
2004-05-17E & PLF	2004-03-17	us	1	opened	<input type="checkbox"/>	Save

[ESRF](#) | [eITPX](#) | [EMBL](#) | [BM14](#) | [SRNE](#) | [MSO](#) | [eScience](#)

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Apache Tomcat/5.0.30



ID14 - EH1


mx-415 TEST  
Logout MCCARTHY E.S.F. Dates: 2005-11-18 to 2005-11-18 User mode

Hutch | Sample changer | Collect | Results | [Equipment status](#)

Available samples:


Sample name	Protein	Acronym	Crystal name	Morphology	Matrix code	Location
-------------	---------	---------	--------------	------------	-------------	----------

Show only the samples inside the sample changer


 Refresh list

Parameters

Directory:	<input type="text" value="/data/id14eh1/external/mx415"/>	Oscillation start (deg):	<input type="text" value="+0.0"/>	Exposure mode:	<input type="text" value="Detachable"/>
Prefix:	<input type="text" value="mx415"/>	Oscillation range (deg):	<input type="text" value="+1.0"/>	Energy (keV):	<input type="text" value="13.275"/>
Run number:	<input type="text" value="1"/>	Overlap (deg):	<input type="text" value="+0.0"/>	Detector resolution (Å):	<input type="text" value="3.0"/>
Template:	<input type="text" value="mx415_1_###.img"/>	Number of images:	<input type="text" value="1"/>	Transmission (%):	<input type="text" value="100"/>
First image #:	<input type="text" value="1"/>	Exposure time (sec):	<input type="text" value="1.0"/>	Detector mode:	<input type="text" value="Unbinned"/>
		Number of passes:	<input type="text" value="3"/>	Comments:	<input type="text"/>

 Collect data

Progress bar: 100% (100/100) Waiting data

Information messages | Details |  Submit feedback

1

2

3



Hutch | Sample changer | Collect | Results | [Help](#)

Status - MOVING

Moving to Basket Location 4 ...



No sample on axis



Selected Matrix

current: 4  
matrix id: 7

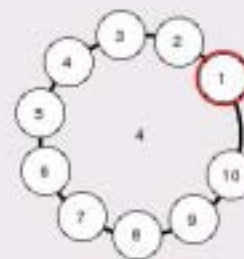
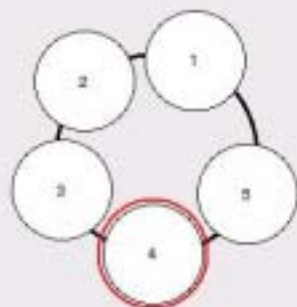
Control panel for Selected Matrix with 'Change' button and 'Back to selected matrix' button.



Selected Matrix

current: 1  
matrix id: 7

Control panel for Selected Matrix with 'Change' button.



Slider control for 'Matrix height (mm)' with a 'Load matrix' button.

Information messages (0) | Details (1) | Submit feedback

Feel free to report any comment about this software; an email will be sent to the people concerned. Do not forget to put your name or email address if you require an answer.

Message



Hutch | Sample changer | Collect | Results | [Feedback](#)

Available samples

Sample name	Protein name	Acronym	Crystal name	Morphology	Matrix code	Location
None	DJ-1	SeDJ-1				
None	EPTPS	EP				
None	HP1230 DNAA binding protein	HP1230				
None	Peptidase	It				
None	Thioredoxin reductase	TR1				
None	Trypsin	typ				
None	beta-lactamase	CMY-10				
Et	thumain bn14	thumw		bi-pyramidal	HA00AA3315	
stal1	Trypsin	typ	noname		HA00AC1908	
stal10	Trypsin	typ	noname		HA00AA4206	
stal2	Trypsin	typ	noname		HA00AA4169	
stal3	Trypsin	typ	noname		HA00AA2679	
stal4	Trypsin	typ	noname		HA00AB4835	
stal5	Trypsin	typ	noname		HA00AA2041	
stal6	Trypsin	typ	noname		HA00AA9990	
stal7	Trypsin	typ	noname		HA00AA9990	

 Show only the samples inside the sample changer


Parameters

Directory: 

Prefa:	<input type="text" value="typ-stal5"/>	Oscillation start (deg):	<input type="text" value="+0.0"/>	Exposure mode:	<input type="text" value=""/>
Run number:	<input type="text" value="1"/>	Oscillation range (deg):	<input type="text" value="+1.0"/>	Energy (keV):	<input type="text" value="13.275"/>
Template:	<input type="text" value="typ-stal5_1_###.img"/>	Overlap (deg):	<input type="text" value="+0.0"/>	Detector resolution (Å):	<input type="text" value="3.088"/>
First image #:	<input type="text" value="1"/>	Exposure time (sec):	<input type="text" value="1.0"/>	Transmission (%):	<input type="text" value=""/>
Number of images:	<input type="text" value="1"/>	Number of passes:	<input type="text" value="3"/>	Detector mode:	<input type="text" value="Unbinned"/>
Comments:					



Inputs

Elapsed time

Remaining time

[Information messages](#) | [Details](#) | [Submit feedback](#)

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Message



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# Interest of ISPyB for MX users today

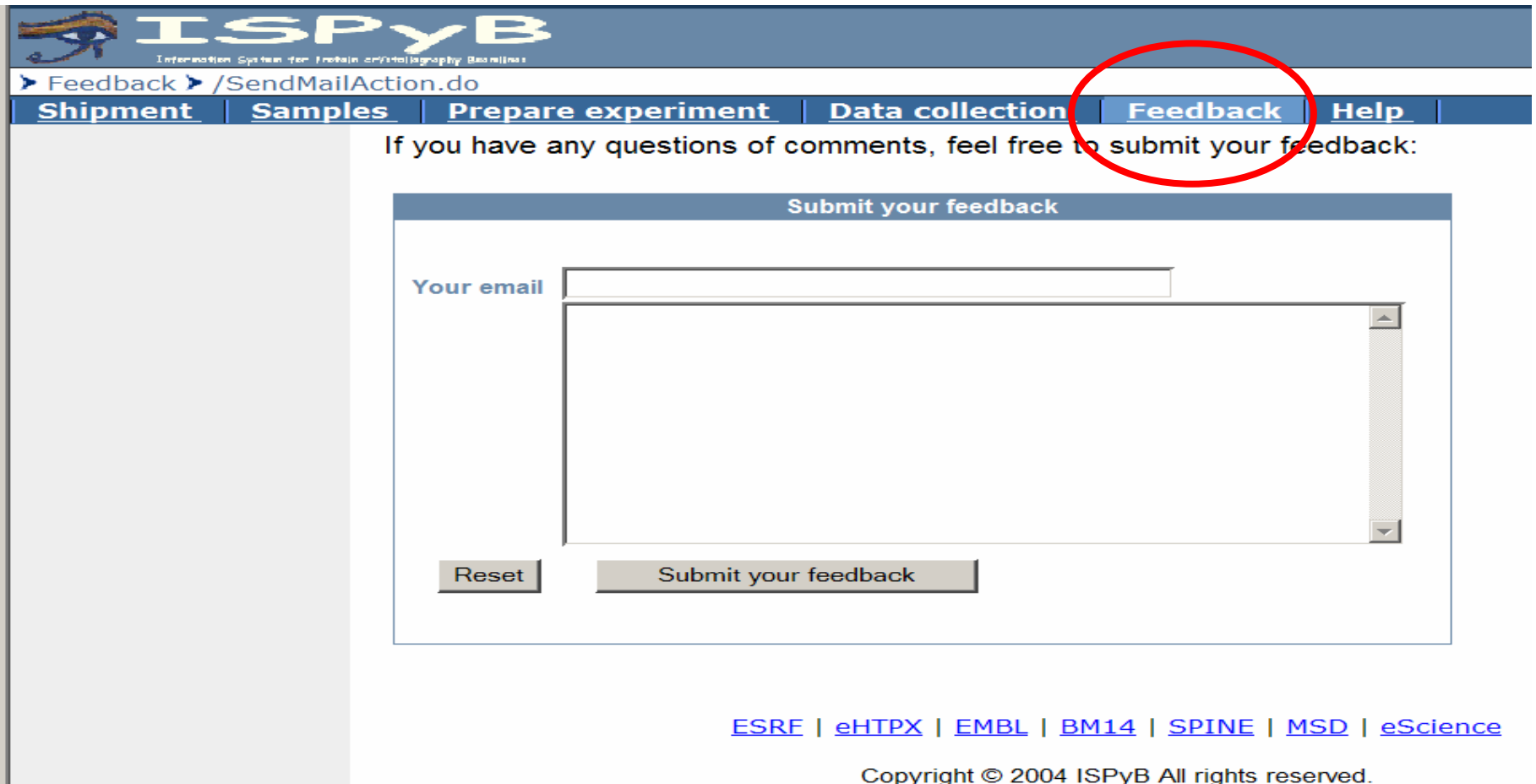
- Electronic logbook :
  - Long term tracking of experiments (stored in the database)
  - Remote tracking by colleagues at home while the experiment is being performed
- Search per protein acronym over last X months
- Shipment form: a way to communicate information from all crystallographers in the lab to the 2 lab-delegates who are doing the experiments at ESRF

# How to use it ?

- **From outside** : <https://ssl.esrf.fr/ispyb> (today 1 log-in at a time from outside on the same account)
- **From inside** : <http://ispyb.esrf.fr:8080/ispyb>
- **Help** on ESRF web pages : <http://www.esrf.fr/UsersAndScience/Experiments/MX/Software/ispyb>

# Contacts

ISPyB : [ispyb@esrf.fr](mailto:ispyb@esrf.fr)



The screenshot shows the ISPyB website interface. At the top, there is a blue header with the ISPyB logo and the text "Information System for Protein Crystallography Beamlines". Below the header, there is a navigation menu with buttons for "Shipment", "Samples", "Prepare experiment", "Data collection", "Feedback", and "Help". The "Feedback" button is circled in red. Below the navigation menu, there is a text prompt: "If you have any questions or comments, feel free to submit your feedback:". Below this prompt, there is a form titled "Submit your feedback". The form contains a text input field labeled "Your email" and a larger text area for feedback. At the bottom of the form, there are two buttons: "Reset" and "Submit your feedback".

ISPyB  
Information System for Protein Crystallography Beamlines

Feedback /SendMailAction.do

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

If you have any questions or comments, feel free to submit your feedback:

Submit your feedback

Your email

Reset Submit your feedback

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

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