

ISPyB user manual



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Part I: Click on a title to directly go to the corresponding page

ISPyB user manual

Part I: Web Interface Description



ISPyB Login

Login

Login

Password (*)

(*) : 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](#).

LoginReset

Use your ESRF experiment number (i.e. mx123, ix123, fx123) and password to log in

General Homepage



Welcome to User : mx415



Latest ISPyB News & Information

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

"Shipment" tab

Click on this tab to deal with the samples you are planning to send by courier.
You will be able to define an electronic shipment, containing electronic dewars and containers
You will be able to enter the samples description based on the protein you have submitted through "samplesheets".
You will be able to retrieve information about the shipments, dewars and containers already submitted.

"Samples" tab

Click on this tab to deal with data concerning your proteins, crystals and samples.
You will be able to create new samples for experiment: samples description will be based on the protein you have submitted through "samplesheets".
You will be able to add/edit a new crystal form for your protein
You will be able to view the lists of your proteins, crystal forms, samples
You will be able to edit the diffraction plans linked to your samples

"Prepare experiment" tab

Click on this tab to prepare the list of samples you want to see during experiment.
You will also need to fill the sample changer manually if you are not using pins with DM codes

"Data collection" 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
You will be able to retrieve information about a particular data collection
You will be able to retrieve information about a particular protein
You will be able to retrieve information about a particular sample

ESRF | eHTPX | EMBL | BM14 | SPINE | MSD

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- 1 Summary of actions you can perform in the various tabs:
- 2 Create, view contacts for your proposal
- 3 Create, view or search a shipment
- 4 Create, view or search samples
- 5 Link a shipment to a sample changer content to populate your sample list in mxCuBE
- 6 View and search your data collections
- 7 Ask questions or give feedback to the ISPyB team
- 8 Find the references to cite when reporting data measured on ESRF MX beamlines
- 9 and 11 Go to information and help pages
- 10 Log out of your ISPyB session

Lab-contacts tab

Lab-contacts

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

▶ Create
 ▪ LabContact
 ▶ View
 ▪ LabContacts

All Lab-contacts						
Card name	Lab name	Lab address	Contact name	Contact first name	Contact phone	Edit / Remove
LabContact1	Lab1	Lab address 1	Contact1	Contact first name1	Contact phone1	
LabContact2	Lab2	Lab address 2	Contact2	Contact first name2	Contact phone2	
LabContact3	Lab3	Lab address 3	Contact3	Contact first name3	Contact phone3	

1

2

3

4

- 1 Previously created lab-contacts
- 2 Create a new lab-contact
- 3 Go back to you lab-contact table (1)
- 4 Edit or remove an existing lab-contact

Shipment tab: Homepage

Shipment

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

Create

- Shipment
- Puck
- CSV upload

View

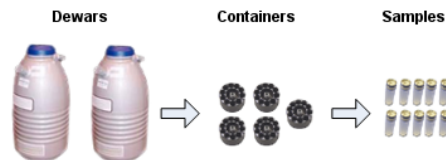
- Shipments
- Dewars

Search

- Shipment
- Dewar



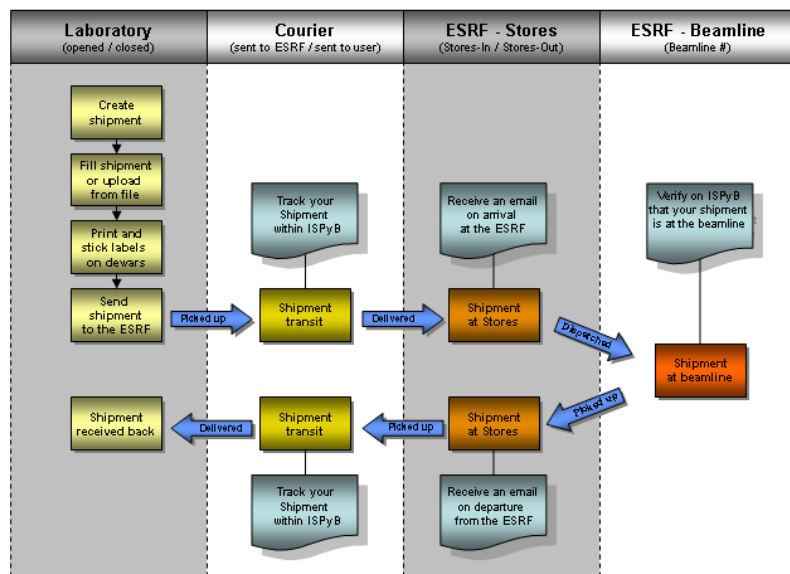
A **Shipment** consists of a set of Dewars which is sent from your home lab to the synchrotron via a courier company. Each dry shipping **Dewar** within the shipment is identified by a label (barcode or sticker). The dewars(s) contains a set of Containers (Baskets or canes). **Containers** (typically Baskets), contain Samples. A **Sample** (Sample Holder) contains the **Crystal**.



Tracking your shipment & contents (Dewars, toolboxes etc) allows you to follow the progress of your shipment from your home Lab to The ESRF. This feature also provides for:

- Generation of Dewar and shipment labels for sending your shipment by courier
- Notification by email of your shipment arrival and departure from The ESRF. Returned shipment notifications also include the courier tracking number to allow you to track the shipment while in transit back to your home laboratory
- Location of your shipment at The ESRF

- Summary of the shipment tracking system put in place at ESRF
- Create a shipment or a puck
- View existing shipments or dewars
- Search for a shipment or a dewar



Shipment tab: Create-> Shipment

Shipment > Create > Shipment

Home Lab-contacts Shipment Samples Prepare experiment Data collection

Create

- Shipment
- Puck
- CSV upload

View

- Shipments
- Dewars

Search

- Shipment
- Dewar

New/Edit Shipment

Details

Creation date: Fri Mar 13 11:22:41 CET 2015

Shipment label: *

Number of dewars: *

Number of other components (i.e. toolbox, laser...):

Beamline / Experiment: *

Comments:

Shipment status: opened

Lab-contacts

Lab-Contact for sending: *

[Creation/Editing of a Lab-Contact card](#)

Return address is identical as sending address (Y/N): ☐

If No, Lab-Contact for Return: *

Courier accounts details for return

These informations are relevant for all shipments.

Courier company for return (if ESRF sends a dewar back):

Courier account:

Billing reference:

Average Customs value of a dewar (Euro):

Average Transport value of a dewar (Euro):

2 Save Save and Edit 3

Details

Creation date: Tue Feb 18 09:08:09 CET 2014

Shipment label: *

Number of dewars: *

Number of other components (i.e. toolbox, laser...):

Beamline / Experiment: No session available

Comments:

Fill-in the different parameters and save to create a new shipment

- 1 An experiment session has to be scheduled and selected in the SMIS system in order to link your shipment with that session
- 2 Save the shipment and redirect you to view that shipment where you can print your tracking label
- 3 Save the shipment and redirect you to the shipment content creation page where you will be able to describe your samples

Shipment tab: Create -> Shipment

Shipment > Create > Shipment

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

Create

- Shipment
- Puck
- CSV upload

View

- Shipments
- Dewars

Search

- Shipment
- Dewar

Shipment

Name test

Creation date 19-02-2014

Status opened

[Back to this Shipment](#)

Upload Shipment from Excel file

test successfully inserted into database.

Help

+

1



Shipment > Create > Shipment

Lab-contacts Shipment Samples Prepare experiment

Create

- Shipment
- Puck
- CSV upload

View

- Shipments
- Dewars

Search

- Shipment
- Dewar

Shipment

Name test

Creation date 19-02-2014

Status opened

[Back to this Shipment](#)

Upload Shipment from Excel file

test successfully inserted into database.

Help

Test +

+

(*) mandatory field for each sample

2



Shipment > Create > Shipment

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

Create

- Shipment
- Puck
- CSV upload

View

- Shipments
- Dewars

Search

- Shipment
- Dewar

Shipment

Name test-3

Creation date 19-02-2014

Status opened

[Back to this Shipment](#)

Upload Shipment from Excel file

test-3 successfully inserted into database.

Help

test again +

puck test +

Save Reset Change sample name automatically

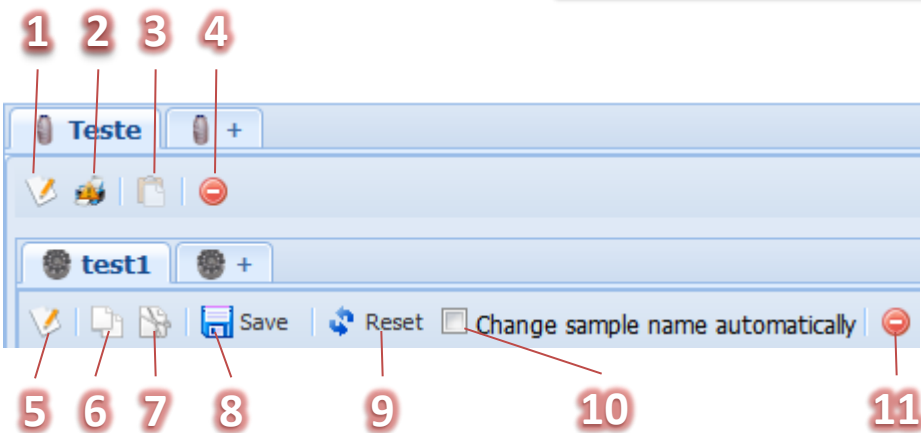
Sample Position	Protein Acronym (*)	Sample Name (*)	Pillarcode	Space Group	Pre-Open resolution	Needed resolution	Oscillator Range	Experiment Type	Unit Cell a	Unit Cell b	Unit Cell c	Unit Cell alpha	Unit Cell beta	Unit Cell gamma	Comments
1								OSC							
2								OSC							
3								OSC							
4								OSC							
5								OSC							
6								OSC							
7								OSC							
8								OSC							
9								OSC							
10								OSC							

(*) mandatory field for each sample

Shipment content creation page:

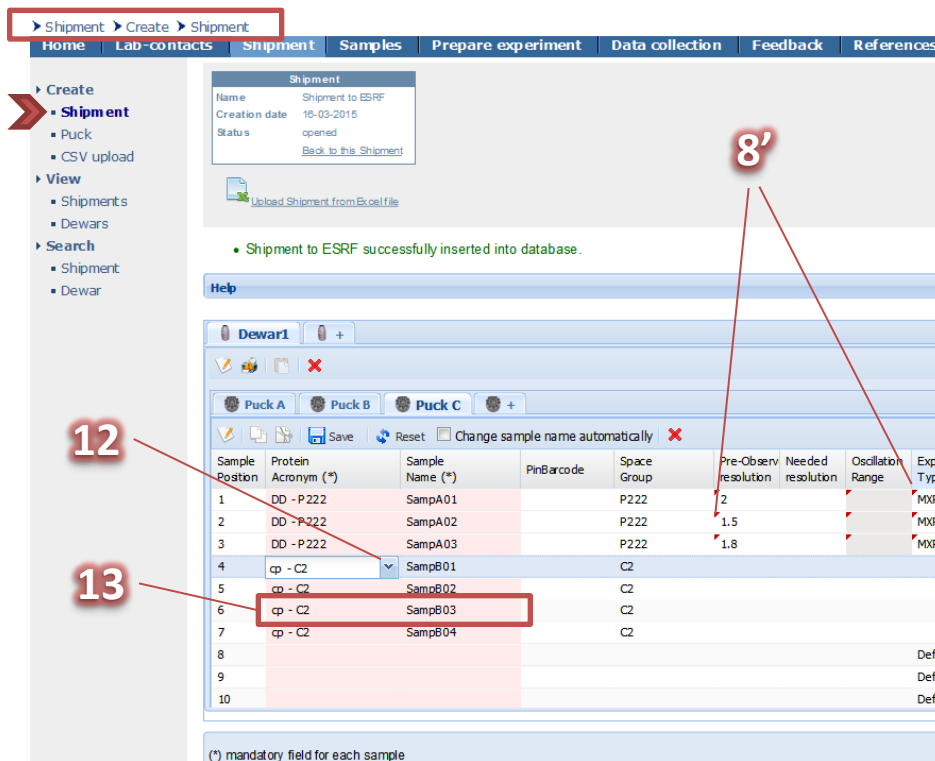
- 1 Add a new dewar to this shipment
- 2 Add and name a new puck
- 3 Fill-in the different cells and save to create a new puck (see next page)

Shipment tab: Create -> Shipment



Fill-in the different cells and save to create a new puck

- 1 Edit the dewar label
- 2 Print your component label
- 3 Paste a copied or cut puck into a new dewar
- 4 Remove this dewar and its content (pucks)
- 5 Edit the puck label
- 6 Copy this puck (or sample 6'). You can then paste it with (3 or 3')
- 7 Cut this puck. You can then paste it with (3)
- 8 Save puck content as it is. Red corner on cells indicate that some information needs to be saved (8')
- 9 Erase all puck content
- 10 When ticked, adds an incremental number to the "sample name"
- 11 Delete puck and its content
- 12 Select your protein acronym from the drop down menu (proteins declared to safety)
- 13 Protein acronym + sample name combination must be unique in a shipment
- 14 Show/Hide help
- 15 Enter here the "simplified molecular-input line-entry system" code. It will be taken into account during small molecule phasing.



Shipment tab: Create-> Puck

Shipment > Create > Puck

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

Create

- Shipment
- Puck**
- CSV upload

View

- Shipments
- Dewars

Search

- Shipment
- Dewar

Puck Information

Shipping:

Dewar:

Puck:

Create Puck

☐ Change sample name automatically

Sample Position	Protein Acronym (*)	Sample Name (*)	PinBarcode	Space Group	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	Comments
1	<input type="text" value="P2"/>			P2	0		0	OSC	0	0	0	0	0	0	
2	<input type="text" value="---"/>							OSC							
3								OSC							
4								OSC							
5								OSC							
6								OSC							
7								OSC							
8								OSC							
9								OSC							
10								OSC							

Create Puck

☐ Change sample name automatically

Fill-in the different cells and save to create a new puck

- 1 Save puck content as it is. Red corner on cells indicate that some informations need to be saved (1')
- 2 Reset puck content
- 3 When ticked, adds an incremental number to the "sample name"
- 4 Select your protein acronym from the drop down menu

Shipment tab: Create -> CSV upload

➤ Shipment ➤ Create ➤ CSV upload

Lab-contacts | Shipment | Samples | Prepare experiment | Data

➤ Create

- Shipment
- Puck
- **▪ CSV upload**

➤ View

- Shipments
- Dewars

➤ Search

- Shipment
- Dewar

Help ⓘ **1**

Submit your .csv file

The file must be a csv file.

File to upload No file selected.

Field separator *

Text separator *

1 Show/Hide help

CSV File example in Excel:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample01	1		90	90	90	90	90	90
2	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample02	2		90	90	90	90	90	90
3	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample03	3		90	90	90	90	90	90
4	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample04	4		90	90	90	90	90	90
5	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample05	5		90	90	90	90	90	90
6	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample06	6		90	90	90	90	90	90
7	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample07	7		90	90	90	90	90	90
8	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	CMY-10	beta-lactamase	P41212	0	sample08	8		90	90	90	90	90	90
9	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	CMY-10	beta-lactamase	P41212	0	sample09	9		90	90	90	90	90	90
10	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	CMY-10	beta-lactamase	P41212	0	sample10	10		90	90	90	90	90	90
11	mx	123	1	ship-20140214	Dewar1	Puck2	3	2.1	0.5	t2	thiolase	C222	0	s01	1		90	90	90	90	90	90
12	mx	123	1	ship-20140214	Dewar1	Puck2	3	2.1	0.5	t2	thiolase	C222	0	s02	2		90	90	90	90	90	90
13	mx	123	1	ship-20140214	Dewar2	Puck3	3	2.1	0.5	t2	thiolase	C222	0	test01	1		90	90	90	90	90	90
14	mx	123	1	ship-20140214	Dewar2	Puck3	3	2.1	0.5	t2	thiolase	C222	0	test02	2		90	90	90	90	90	90

Upload your CSV file to create a new shipment

Shipment tab: View -> Shipments

Shipment > View > Shipments

Lab-contacts

Shipment

Samples

Prepare experiment

Data collection

Feedback

References

Help

Logo

Create

- Shipment
- Puck
- CSV upload

View

- Shipments
- Dewars

Search

- Shipment
- Dewar

Shipments

Edit	Shipment Name	Creation date	Expected at ESRF	Sending details	Return details	# components (# samples)	View Components	View Samples	Comments	Status	History	Actions
	test	07-07-2014				1 (0)						
	tes soleil	24-06-2014				3 (0)						
	ship-20140602	02-06-2014				1 (2)						
	ship-20140523	23-05-2014				1 (1)				processing		Processing
	WF-realXtals	24-03-2014				1 (50)				at ESRF		

1

2

3

4

5

6

7

8

9

10

In the Shipment tab-> View -> Shipments page you can :

- 1 Edit an existing shipment (attach it to another session, change the transport details or comments)
- 2 and 4 List the component details of that shipment
- 3 List the number of components and samples already registered for this shipment
- 5 View all samples of that shipment
- 6 Comments that can be edited during shipment creation or in (1)
- 7 View your shipment status (sent to ESRF, at ESRF, not complete or processing)
- 8 View the shipment information and dewar history
- 9 Actions that can be performed on your shipment: add a dewar, upload its content from XLS files, edit its content, put it in 'sent to ESRF' mode. These icons are replaced by **processing** if it has been used on the beamline
- 10 Delete that shipment If you have data collected for this shipment, this will delete them!!

Shipment tab: View -> Dewars

Shipment View Dewars

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

Create

- Shipment
- Puck
- CSV upload

View

- Shipments
- Dewars**

Search

- Shipment
- Dewar

Comp. name	Type	Ship. name	Comments	Barcode	Sending details	Exp. date	Beamline	# samples	Courier/ tracking # TO ESRF	Component status	Location	View Containers	View Samples	Return details	Courier/ tracking # FROM ESRF	History	Comp. labels
Dewar1		test		ESRF0306751				0		opened							
case1		tes_soleil		ESRF306713				0		opened							
		tes_soleil		ESRF306712				0		opened							
test		tes_soleil		ESRF306711				0		opened							

1 2 3 4 5 6 7

In the Shipment tab -> View -> Dewars page you can :

- 1 View the type of component included in all your shipments (dewars or other)
- 2 View the barcode issued for that shipment for tracking purpose (tracking sheet printable from (6))
- 3 Check your component status (opened, ready to go, at ESRF, sent to user, closed)
- 4 List the pucks of this dewar
- 5 List the samples of dewar
- 6 View your component history
- 7 Print you component label

Shipment View Shipments

Lab-contacts Shipment

Create

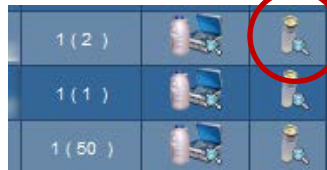
- Shipment
- Puck
- CSV upload

View

- Shipments**
- Dewars

Search

- Shipment
- Dewar



Shipment tab:
View -> Shipments or Dewars
-> View samples



Export as PDF(sort by dewar/container/location)



Export as PDF(sort by acronym/sample name)

Samples																						
Protein	Space Group	Sample name	Smp code	Shipment	Dewar	Container	Loc. in cont.	Cell a	Cell b	Cell c	Cell alpha	Cell beta	Cell gamma	Crystal comments	Already observed resol.	Required resol.	Minimal resol.	Sample comments	Edit sample	Sample status	Data Collections	Data CollectionGroups
CER	P212121	sampA01	HA00AQ8595	WF-realXtals	dewar1	CB340A-Steph1	1	55.0	63.0	69.0	90.0	90.0	90.0			1.5						
CER	P212121	sampA02	HA00AP6006	WF-realXtals	dewar1	CB340A-Steph1	2	55.0	63.0	69.0	90.0	90.0	90.0			2						
CER	P212121	sampA03	HA00AQ8103	WF-realXtals	dewar1	CB340A-Steph1	3	55.0	63.0	69.0	90.0	90.0	90.0			3						
CER	P212121	sampA04	HA00AQ8573	WF-realXtals	dewar1	CB340A-Steph1	4	55.0	63.0	69.0	90.0	90.0	90.0			1.5						
CER	P212121	sampA05	HA00AQ8114	WF-realXtals	dewar1	CB340A-Steph1	5	55.0	63.0	69.0	90.0	90.0	90.0			2						
CER	P212121	sampA06	HA00AP6015	WF-realXtals	dewar1	CB340A-Steph1	6	55.0	63.0	69.0	90.0	90.0	90.0			3		sans cryo				
CER	P212121	sampA07	HA00AQ8584	WF-realXtals	dewar1	CB340A-Steph1	7	55.0	63.0	69.0	90.0	90.0	90.0					sans cryo				
CER	P212121	sampA08	HA00AP9755	WF-realXtals	dewar1	CB340A-Steph1	8	55.0	63.0	69.0	90.0	90.0	90.0					sans cryo				
CER	P212121	sampA09	HA00AQ8580	WF-realXtals	dewar1	CB340A-Steph1	9	55.0	63.0	69.0	90.0	90.0	90.0					sans cryo				
CER	P212121	sampA10	HA00AB6186	WF-realXtals	dewar1	CB340A-Steph1	10	55.0	63.0	69.0	90.0	90.0	90.0					sans cryo				
CER	P212121	sampB01	HA00AQ6589	WF-realXtals	dewar1	CB340A-Steph1	1	55.0	63.0	69.0	90.0	90.0	90.0			1.8						
CER	P212121	sampB02	HA00AC6788	WF-realXtals	dewar1	CB340A-Steph1	2	55.0	63.0	69.0	90.0	90.0	90.0			2		Long pin - Lucid fails				
CER	P212121	sampB03	HA00AQ6927	WF-realXtals	dewar1	CB340A-Steph1	3	55.0	63.0	69.0	90.0	90.0	90.0			2.5						

1

2

3

4

5

6

7

From the Shipment-> View -> Shipments page you can go to a summary page of the samples registered in one shipment :

- Click on link to open the sample detail page
- Click on link to open the shipment detail page
- Click on link to view all the samples in this dewar
- Parameters and comments previously entered when creating the sample

- Edit or delete this sample
- View the data collections
- View collection summary by group (sample name, experiment type...)

Shipment tab: Search

► Shipment ► Search ► Shipment

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

► Create

- Shipment
- Puck
- CSV upload

► View

- Shipments
- Dewars

► Search

- **Shipment**
- Dewar

Search Shipping

Shipment label :

Creation date between DD-MM-YYYY :

and DD-MM-YYYY :

You may use the * character to do a search with an incomplete field.

[ESRF](#) | [eHTPX](#) | [EMBL](#) | [BM14](#) | [SPINE](#) | [MSD](#) | [eScience](#)

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► Shipment ► Search ► Dewar

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

► Create

- Shipment
- Puck
- CSV upload

► View

- Shipments
- Dewars

► Search

- Shipment
- **Dewar**

Search Dewars

Label

Comments

Experiment date between DD-MM-YYYY :

and DD-MM-YYYY :

Status

Location

You may use the * character to do a search with an incomplete field.

[ESRF](#) | [eHTPX](#) | [EMBL](#) | [BM14](#) | [SPINE](#) | [MSD](#) | [eScience](#)

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Use these pages to search a particular shipment or a dewar

Samples tab: Homepage

The screenshot shows the 'Samples' tab selected in a navigation bar. The left sidebar contains a menu with the following items: 'Create' (with sub-items 'New sample' and 'New crystal form'), 'View' (with sub-items 'Proteins and crystal forms' and 'Unassigned Samples'), 'Search' (with sub-items 'Protein' and 'Sample'), and 'Update Database'. On the right, the main content area is titled 'What you can do in the samples pages' and contains sections for 'Create', 'View', 'Search', and 'Update Database'. Red callout numbers are placed as follows: 1 points to the main content area; 2 points to 'New sample'; 3 points to 'Proteins and crystal forms'; 4 points to 'Protein'; 5 points to 'Update Database'.

1 Summary of the actions you can perform under the samples tabs

2 Create a sample or a crystal form for a protein

3 View existing protein crystal forms or unassigned samples (not attached to a shipment)

4 Search for a protein (by its acronym) or a sample (by its barcode or name)

5 Retrieve the protein acronyms from your sample sheets newly submitted in the SMIS database

Samples tab: Create -> New sample

1'

Use this form to create a new sample related to your protein

1 If you don't find your protein in the list on the left, update the database (1')

1

Samples tab: Create -> New crystal form

► Samples ► Create ► New crystal form

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

► Create

- New sample
- **New crystal form**

► View

- Proteins and crystal forms
- Unassigned Samples

► Search

- Protein
- Sample

1' → Update Database

Create a new Crystal Form

Please select a Protein Acronym **1**
this field is required

Geometry Class

- Primitive triclinic
- Primitive monoclinic
- Centred monoclinic
- Primitive orthorhombic
- C-centred orthorhombic
- I-centred orthorhombic
- F-centred orthorhombic
- Primitive tetragonal
- I-centred tetragonal
- Primitive trigonal
- Primitive hexagonal
- Rhombohedral
- Primitive cubic
- I-centred cubic
- F-centred cubic
- Unknown

Space Group

a b c
Alpha Beta gamma

Morphology Color

Crystal size X Crystal size Y Crystal size Z

Comments

Reset Save

Use this form to create a new crystal form related to your protein

1 If you don't find your protein here, update your ISPyB database (**1'**)

Samples tab: View-> Protein and crystal forms

► Samples ► View ► Proteins and crystal forms

Lab-contacts Shipment **Samples** Prepare experiment Data collection Feedback References Help Lo

- Create
 - New sample
 - New crystal form
- View
 - **Proteins and crystal forms**
- Search
 - Protein
 - Sample
- Update Database

Click on the acronym, or on the space group to see the samples attached to corresponding acronym, space group.

Proteins and Crystal Forms List																
	Protein Name		Protein Acronym	New Crystal Form	SpaceGroup	A	B	C	Alpha	Beta	Gamma	Comments	Edit	Delete	PDB File	Data Collections
	test		test1		Undefined	32.016	33.281	48.002	77.97	70.54	61.28					View
	test					108.666	180.159	101.144	90.0	110.3	90.0					View
	Mnth		Mnth		R32	0.0	0.0	0.0	0.0	0.0	0.0					View
	PA0688		PA0		P21	0.0	0.0	0.0	90.0	0.0	90.0					View

1

2

3

4

5

Allows you to view all proteins and their associated crystal forms

- 1 Create a new crystal form for that protein
- 2 Edit this crystal form
- 3 Delete this crystal form
- 4 Upload the corresponding PDB file (for Autoprocessing purposes)
- 5 View all the data collections measured for that crystal form of that protein

Samples tab: Search -> Protein or sample

► Samples ► Search ► Protein

Lab-contacts | Shipment | **Samples** | Prepare experiment | Data collection | Feedback

- Create
 - New sample
 - New crystal form
- View
 - Proteins and crystal forms
 - Unassigned Samples
- Search
 - **Protein**
 - Sample
- Update Database

Search Protein

Acronym

You may use the * character to do a search with an incomplete Acronym.

► Samples ► Search ► Sample

Lab-contacts | Shipment | **Samples** | Prepare experiment | Data collection | Feedback

- Create
 - New sample
 - New crystal form
- View
 - Proteins and crystal forms
 - Unassigned Samples
- Search
 - Protein
 - **Sample**
- Update Database

Search Sample

Name

Datamatrix Code

You may use the * character to do a search with an incomplete Name.

[ESRF](#) | [eHTPX](#) | [EMBL](#) | [BM14](#) | [SPINE](#) | [MSD](#) | [eScience](#)

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Use these pages to search for a particular protein or a sample

Samples tab: Update Database

The screenshot shows the ISPyB web interface. At the top, a navigation bar contains the following tabs: Lab-contacts, Shipment, Samples, Prepare experiment, Data collection, Feedback, References, and Help. The 'Samples' tab is currently selected. Below the navigation bar, a left sidebar contains a menu with the following items: Create (with sub-items New sample and New crystal form), View (with sub-items Proteins and crystal forms and Unassigned Samples), Search (with sub-items Protein and Sample), and Update Database. A red arrow points to the 'Update Database' item. The main content area displays the text: "When creating a new sample, if some protein acronyms are missing in the list, you can get them by updating ISPyB database (this may take a few minutes)." At the bottom of the page, there is a footer with the text: "ESRF | eHTPX | EMBL | BM14 | SPINE | MSD | eScience" and "Copyright © 2004 ISPyB All rights reserved."

► Samples ► Update Database

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

► Create

- New sample
- New crystal form

► View

- Proteins and crystal forms
- Unassigned Samples

► Search

- Protein
- Sample

► **Update Database**

When creating a new sample, if some protein acronyms are missing in the list, you can get them by updating ISPyB database (this may take a few minutes).

[ESRF](#) | [eHTPX](#) | [EMBL](#) | [BM14](#) | [SPINE](#) | [MSD](#) | [eScience](#)

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Click on “updating ISPyB database” to retrieve protein acronyms from recent submitted safety sheets in the SMIS database (synchronisation with SMIS database)

Prepare experiment tab

Prepare experiment

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

Select Dewars

- Last dewars
- All dewars

Fill sample changer

View

- Selected dewars

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- Associate data collections to samples in mxCuBE.



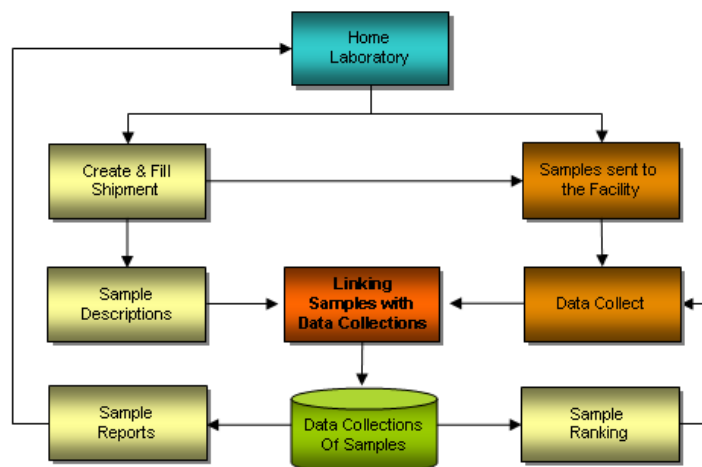
First step: Select the dewars

5



Linking Samples to Data Collection: how does it help my experiment?

Linking Samples of your Shipment (sample descriptions) with Crystals in the Sample changer (physical samples) will allow you to associate the Data Collections made on these crystals to their Sample description. Then, you will be able to make Sample Ranking or to make reports that can be processed by your LIMS.



1 Describes the purposes of the “prepare experiment” tab (to view your ISPyB samples within the data collection GUI mxCuBE)

2 and 5 Select the dewar you want to put in processing from a shortlist (last 60 days)

2' Same as 2 but showing all dewars in that user account

3 Specify directly where samples are located in the sample changer

6 View dewar(s) selected in 2.

Prepare experiment pages – Select Dewars

Prepare experiment > Select Dewars > Last dewars

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

















- ▶ Select Dewars
 - ▶ Last dewars
 - All dewars
 - ▶ Fill sample changer
 - ▶ View
 - Selected dewars

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 Damatrix codes)
- 3- In MxCuBe, link the samples in the container to the crystals in the Sample Changer.

Next step: Fill the sample changer — 6

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

Select dewars for processing														
 Ship. name	 Creation date	 Comp. name	Type	Comments	Barcode	 Exp. date	 Beamline	# containers (# samples)	Local contact	 Dewar status	 Location	View Containers	View Samples	Select for processing
ship-20140523	23-05-2014	Dewar1						1 (1)		processing				<button>Deselect</button>
test	07-07-2014	Dewar1			ESRF0306751			1 (0)		opened				<button>Select</button>
tes_soleil	24-06-2014	case1			ESRF0306713			0 (0)		opened				<button>Select</button>

1

2

3

4

5

In this tab dewars not selected appear in blue and dewars already selected appear in orange

- 1 View the type of component included in your shipment (dewar or toolbox)
- 2 Check your component status (opened, ready to go, at ESRF, sent to user, closed)
- 3 List the pucks of that dewar
- 4 List the samples of that dewar
- 5 Select or deselect this dewar for sample changer filling
- 6 Click to define the positions of the pucks in the sample changer

Tip: If you do not see a dewar that you have already created, click on "All dewars"

Prepare experiment tab: Fill sample changer

► Prepare experiment ► Fill sample changer

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

► Select Dewars

- Last dewars
- All dewars

► Fill sample changer

► View

- Selected dewars

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

3

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-20140206id29	06-02-2014	Dewar1	ESRF0306223	Puck1	Puck	10	6	ID29	1
<div>Save</div>									

2

1

- 1 Enter the beamline location and the sample changer position of the puck
- 2 Save the pucks location
- 3 Click here to view a guide on how to view your selected samples in MxCuBE

Prepare experiment tab: View

Prepare experiment > View > Selected dewars

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

Select Dewars

- Last dewars
- All dewars

Fill sample changer

View

- Selected dewars

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 Damatrix codes)

3- In MxCuBe, link the samples in the container to the crystals in the Sample Changer.



Next step: Fill the sample changer

6

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

Select dewars for processing												
Ship. name	Creation date	Comp. name	Type	Comments	Barcode	Exp. date	Beamline	# containers (# samples)	Local contact	Dewar status	Location	Select for processing
ship-20140523	23-05-2014	Dewar1						1 (1)		processing		

1 results found

1

2

3

4

5

Here you can view the list of the previously selected dewars

- 1 and 3 List the content (pucks) of that dewar
- 2 Check your dewar status (opened, ready to go, at ESRF, sent to user, processing, closed)
- 4 View the samples registered in this dewar
- 5 Select or deselect this dewar to view it in MxCuBe (beamline control software)
- 6 Click to define the positions of the pucks in the sample changer

Data collection tab

► Data collection ► View all sessions

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

- 1 View last sessions
- 2 View all sessions
- 3 Search data collections

Search Sessions ▼

All sessions										
Start Date	End Date	Beamline	Local contact	# Shifts	Comments	Edit	View session report	View collections groups	View collections	SMIS A-Form
26-06-2014	27-06-2014	ID29	POUDEVIGNE E	2						A-Form
28-04-2014	29-04-2014	ID23-1	CARPENTIER E	2						A-Form
18-03-2014	19-03-2014	ID23-1	MONACO S	2						A-Form
17-02-2014	18-02-2014	ID23-1	POPOV A	2						A-Form
13-12-2013	15-12-2013	ID23-1	MUELLER DIECKMANN C	2						A-Form
30-10-2013	01-11-2013	ID23-1	POPOV A	2						A-Form
05-09-2013	07-09-2013	ID23-1	POPOV A	2						A-Form
17-06-2013	19-06-2013	ID23-1	POPOV A	1						A-Form
15-04-2013	17-04-2013	ID23-1	DE SANCTIS D	2						A-Form
21-02-2013	23-02-2013	ID23-1	GORDON E	2						A-Form
03-12-2012	05-12-2012	ID23-1	ALI S	2						
13-09-2012	14-09-2012	ID23-1	RUSSI S	1						
22-06-2012	23-06-2012	ID23-1	LEONARD G	1						
20-06-2012	22-06-2012	ID23-1	FLOT D	1						
03-10-2011	05-10-2011	ID23-1	LEONARD G	1						
29-06-2011	01-07-2011	ID23-1	MONACO S	1						
09-05-2011	11-05-2011	ID23-1	FERRAZ LEAL R	2						
10-03-2011	12-03-2011	ID23-1	CARPENTIER E	2						
02-02-2011	04-02-2011	ID23-1	MCCARTHY A	2						
09-12-2010	10-12-2010	ID23-2		3	Session created by the BCM					
						1 2 3 4 >>				Go to page

- 1 View your 20 last sessions
- 2 View all your sessions
- 3 Search for a specific data collection or a set of data collections
- 4 Add comments to this session
- 5 View reports (parameters, snapshot, autoproccessing...) for a specific session

- 6 View collection summary by sample
- 7 View a chronological summary of your collects and detailed autoproccessing results
- 8 View the A-form (SMIS) corresponding to that session
- 9 Filter the sessions by date and/or beamtime
- 10 and 11 View a specific page of the session list

Data collection tab: view session report

Data collection

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

View last sessions
View all sessions
Search data collections

Selected Session
Start Date: 18-07-2014
BeamLine: ID29 +33476882905
[Back to this session](#)
[Back to sessions](#)

Session Information

Local Contact: LEONARD G
Comments:
Dewar Transport:
Data backup & Express delivery France:
Data backup & Express delivery Europe:

Save

Session Statistics

Nb Collect: 57
Nb Test: 68
Nb Energy Scan: 0
Nb XRF Spectra: 0

Reports

General report:

[WE](#) [PDF](#)

Screening report:

[WE](#) [PDF](#)

Parameters

Results

Sort Ascending
Sort Descending
Columns
Group by this field
Show in groups

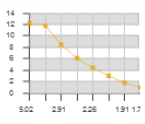
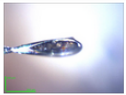
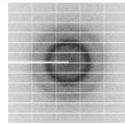
Session

Save Comments View All DataCollection

Experiment Type Image Prefix Run# Parameters Results Image Thumbnail Crystal snapshot Graph Comments

Start time: 17:45:52
18-07-2014 (1 item)

OSC CP232A10_w1 1 Nb images: 1600 Exp. time: 0.05 s Phi range: 0.10 ° Flux: 1.37E12 ph/sec Detector resolution: 1.40 Å Transmission: 49.76 Wavelength: 0.977 Å Total expo time: 80.00 s
EDNA dp GrenADES fp GrenADES pp
Space Group: C 1 2 1
Completeness:



1 Add comments about this session and save

2 Download collection reports of different kind and of various formats

3 Click on the right end of the title row to set the parameters grouping/sorting

NB: You can order the columns as you wish by dragging the title where you want

4 Expand/ collapse all lines or clear the parameters grouping

5 View chronological data collection for that session and basic autoproccessing results

6 Experiment type (OSC=standard collection, characterisation...)

7 Click here to view all the details of this experiment (parameters, autoproccessing results...)

8 Experiment parameters

9 View collection autoproccessing status and results

10 Click on the diffraction thumbnail to view full size image

11 Click on the crystal snapshot to view full size image

12 Click on the analytical graph to view full size image

13 Add comments about this data collection and save (13')

Data collection tab: view collections groups

View collections groups

► Data collection

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

► View last sessions
► View all sessions
► Search data collections

Selected Session

Start Date 20-02-2014
BeamLine ID29 +33476882805
[Back to this session](#)
[Back to sessions](#)

Session Information

Local Contact:
Comments:
Save

Session Statistics

Nb Collect: 98
Nb Test: 8
Nb Energy Scan: 0
Nb XRF spectra: 0

DataCollectionGroups EnergyScans XRF spectra

Save Comments View DataCollection for all groups Expand All Collapse All Clear Grouping

Workflow	Experi Type	Protein Acronym	Image Prefix	Run No	Sample position	Start Time	Comments	Nb Data Collect	Nb images	View Collections
Sample name: (15 Items)										
XrayCentering	Helical			(1)		20-02-2014 16:...		4	4	
XrayCentering	Helical			(1)		20-02-2014 16:...		5	4	
	OSC			(1)		20-02-2014 16:...		7	20	
	OSC			(1)		20-02-2014 16:...		7	20	
	OSC			(1)		20-02-2014 16:...		7	900	
	Helical			1	(1)	20-02-2014 16:...		1	100	

- 1 Save comments
- 2 Click to view the data collections associated with that of that workflow (collects, images, results)
- 3 View chronological data collection for that session and basic autoprocessing results
- 4 View your collections
- 5 Energy scans for that session
- 6 XRF spectra for that session

Data collection tab: view collections

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

View last sessions
View all sessions
Search data collections

Selected Session
Start Date 28-06-2014
BeamLine ID29 +33476882805
[Back to this session](#)
[Back to sessions](#)

Data Collection info...

1 Reports
General report:
Screening report:

2 Parameters
Ignore RSymm in the low resolution shell over: 10
Ignore I / Sigma in the low resolution shell under: 1
Update

3 References
When reporting data collected on ID29 please cite the appropriate references
ID29
EDNA
Workflow
MxCuBE
ISPyB
BEST
AutoProcessing
Download as BibTeX

4

11 Save Experiment Parameters Rank EDNA Expand All Collapse All Clear Grouping

Image Prefix	Run No	Experiment Type	Protein Abstr	Start time	# images	Experiment Parameters	Status	Space Group	Completeness	Resolution	Rsymm Inner Outer Overall	Unit cell a, b, c alpha, beta, gamma	Sample Ranking	Skip	Comments	Download autoproc files
ref-308	1	Chara...		26-06-2014 18:54:02	2			C2		2.93		271.90, 49.07, 106.39 90.00, 92.61, 90.00	<input checked="" type="checkbox"/>	<input type="checkbox"/>		
ref-307	2	Chara...		26-06-2014 18:45:52	2			P222		2.41		40.69, 49.09, 103.69 90.00, 90.00, 90.00	<input checked="" type="checkbox"/>	<input type="checkbox"/>		
ref-307	1	Chara...		26-06-2014 18:43:09	2					0.00			<input type="checkbox"/>	<input type="checkbox"/>		
306_w1	2	OSC		26-06-2014 18:35:52	1800			C 2 2 2	100 - 4.95 2.38 - 2.3 100 - 2.3	7.3 153.8 18.1	87.80, 209.30, 50.10 90.00, 90.00, 90.00	<input type="checkbox"/>	<input type="checkbox"/>			
306_w1	1	OSC		26-06-2014 18:31:17	1800			C 2 2 2	100 - 5.0 2.77 - 2.2 100 - 2.67	9.2 273.7 26.4	87.70, 208.60, 50.00 90.00, 90.00, 90.00	<input type="checkbox"/>	<input type="checkbox"/>			

5 6 7 8 9 10

- 1 Download reports for that session in various formats
- 2 Tunable parameters for the autoprocessing results summary display
- 3 References to quote for the publication of your results collected at ESRF
- 4 Show/ Hide data collection info
- 5 Show experiment parameters table (wavelength, transmission, exposure time, Phi start, Phi range and detector resolution)

- 6 View collection status (snapshot, data collection, indexing, autoprocessing)
- 7 Best autoprocessing summary
- 8 Select that characterisation for ranking
- 9 Start sample ranking
- 10 Download the autoprocessing files for that collect
- 11 Save your comments

Data collection tab: Search data collections

► Data collection ► Search data collections

Lab-contacts | Shipment | Samples | Prepare experiment | **Data collection**


► View last sessions
► View all sessions
► **Search data collections**


Search data collection

Sample name:

Protein acronym:

Beamline:

Experiment date between DD-MM-YYYY: 

and DD-MM-YYYY: 

Min number of images:

Max number of images:

Image prefix:

Max Data Collections retrieved:

You may use the * character to do a search with an incomplete Name.

Use this form to look for specific data collection(s)

Feedback tab

Feedback

Lab-contacts

Shipment

Samples

Prepare experiment

Data collection

Feedback

References

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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Use this form to give us feedback. We value your opinion and advices on ISPyB and we will use your feedback to improve its operation. We will be happy to help you use ISPyB if necessary.

References tab

References

Lab-contacts

Shipment

Samples

Prepare experiment


Data collection

Feedback


References


When reporting data from the ESRF MX beamlines please cite the appropriate references:


 [ID23-1](#)

 [ID23-2](#)


 [ID29](#)

 [EDNA](#)

 [Workflow](#)

 [MxCuBE](#)

 [ISPyB](#)

 [BEST](#)

 [X-ray fluorescence spectra](#)

 [AutoProcessing](#)

 [Mesh scan](#)

Download as BibTeX

[ESRF](#) | [eHTPX](#) | [EMBL](#) | [BM14](#) | [SPINE](#) | [MSD](#) | [eScience](#)

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List the references to quote when you report data from the ESRF MX beamlines


Help tab

Help

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

What is ISPyB?

News web pages

 [Latest ISPyB News & Information](#)

Help web pages

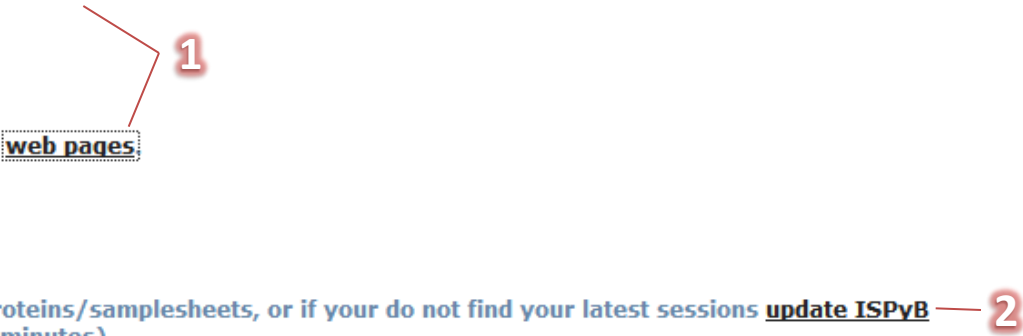
You may find some help on our [web pages](#)

Database update

If you do not find your latest proteins/samplesheets, or if you do not find your latest sessions [update ISPyB database](#) (this may take a few minutes).

ESRF | [eHTPX](#) | [EMBL](#) | [BM14](#) | [SPINE](#) | [MSD](#) | [eScience](#)

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- 1 Redirection to our web pages where you will find News, information and help pages
- 2 Click on this link to update the ISPyB database with new proteins (safety sheets) or new session which are stored in the SMIS database (an automatic update takes place every night)

ISPyB user manual

Part II: How to's



How to:

Track your shipment through ISPyB

Procedure summary

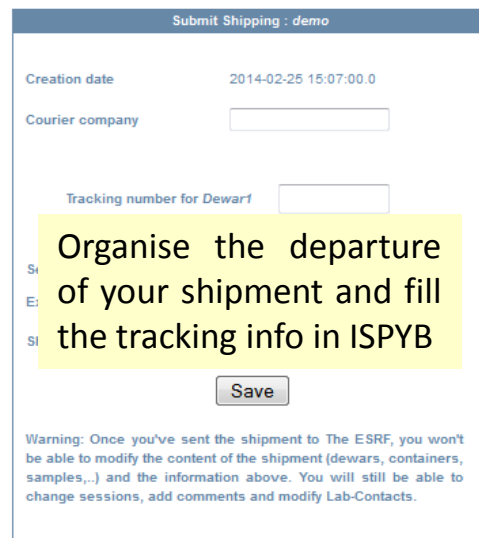


Create a Lab-contact



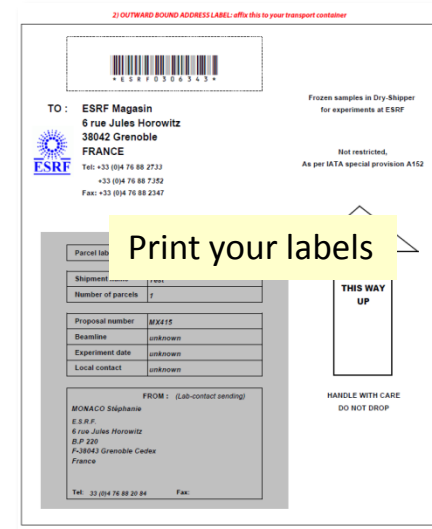
Create a shipment in ISPYB

Tracking your shipment
& contents (Dewars,
toolboxes etc) allows
you to follow the
progress of your
shipment from your
home Lab to ESRF and
back



Organise the departure
of your shipment and fill
the tracking info in ISPYB

Warning: Once you've sent the shipment to The ESRF, you won't be able to modify the content of the shipment (dewars, containers, samples,...) and the information above. You will still be able to change sessions, add comments and modify Lab-Contacts.



Print your labels

How to: Track your shipment through ISPyB *Create a lab contact*

=> If your lab-contact already exists please go directly to step 2

Lab-contacts > Create > LabContact

Lab-contacts | Shipment | Samples | Prepare experiment

► Create

- LabContact

► View

- LabContacts

New/Edit LabContact

Scientist name

Scientist firstname

• No match found in SMIS Database.

New/Edit LabContact

Scientist name

Scientist firstname

Select the scientist contact

Scientist name	Scientist first name	Lab name	Action
Monaco	Stéphanie	ESRF	Select
Monaco	Stéphanie	ESRF	Select
Monaco	Stéphanie	ESRF	Select
Monaco	Stéphanie	ESRF	Select

• (The following lab-contact card already exists)

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 ESRF sends a dewar back)

Courier account

Billing reference

Average Customs value of a dewar (Euro)

Average Transport value of a dewar (Euro)

- 1 Fill in scientist name and search the SMIS database for that particular proposal
- 2 If not found: select one person in your group and go to (3)
- 3 If found: fill-in & save

NOTE: this needs to be done only ONCE for your proposal and for your LAB address

How to:

Track your shipment through ISPyB

Create a shipment

► Shipment ► Create ► Shipment

Lab-contacts | Shipment | Samples | Prepare experiment | Data collection | Fee

► Create

- Shipment
- Puck
- CSV upload

► View

- Shipments
- Dewars

► Search

- Shipment
- Dewar

New/Edit Shipment

Details

Creation date: Tue Feb 25 12:45:46 CET 2014

Shipment label: *

Number of dewars: *

Number of other components (i.e. toolbox, laser...): 0

Beamline / Experiment: 25-02-2014 ID23-1 *

Comments:

Shipment status: opened

Lab-contacts

Lab-Contact for sending: select a contact card *

[Creation/Edition of a Lab-Contact card](#)

Return address is identical as sending adress (Y/N): ☐

If No, Lab-Contact for Return: select a contact card *

Courier accounts details for return

These informations are relevant for all shipments.

Courier company for return (if ESRF sends a dewar back):

Courier account:

Billing reference:

Average Customs value of a dewar (Euro):

Average Transport value of a dewar (Euro):

Save Save and Edit

- 1 Fill in details with components & 2 dewars
- 2 Save & edit

NOTE: if in the field Beamline/Experiment "No session available" appears, please contact deborah.davison@esrf.fr to check that your experiment is scheduled in the SMIS system – If it is already scheduled but this was done during the day of the shipment creation, update ISPYB db with SMIS db info by clicking on 'Help tab' and **update ISPYB database** link

How to:

Track your shipment through ISPyB

Print your labels

➤ Shipment ➤ Create ➤ Shipment

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

➤ Create

- Shipment
- Puck
- CSV upload

➤ View

- Shipments
- Dewars

➤ Search

- Shipment
- Dewar

1'

Shipment

Name: demo
Creation date: 25-02-2014
Status: opened
[Back to this Shipment](#)

Upload Shipment from Excel file

Help

Dewar1

(*) mandatory field for each sample

1) DEWAR LABEL: affix this to your DEWAR

ESRF

* E S R F 0 3 0 6 3 4 9 *

Parcel label	Dewar1
Shipment name	demo
Number of parcels	1
Proposal number	MX415
Laboratory name	E.S.R.F.
Local contact	

2) OUTWARD BOUND ADDRESS LABEL: affix this to your transport container

2

TO : ESRF Magasin
6 rue Jules Horowitz
38042 Grenoble
FRANCE
Tel: +33 (0)4 76 88 2733
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	demo
Number of parcels	1
Proposal number	MX415
Beamline	ID23-2
Experiment date	25-02-2014
Local contact	

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 84 Fax:

3) RETURN BOUND ADDRESS LABEL: include in your shipment, either behind the outbound address label or in the shipment container

3

TO : (Lab-contact for return)
MONACO Stéphanie
Tel: +33 (0)4 76 88 20 84 Fax:
E.S.R.F.
6 rue Jules Horowitz
B.P. 220
F-38043 Grenoble Cedex
France

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	demo
Number of parcels	1
Proposal number	MX415
Courier company	
Courier account	undefined
Billing reference	undefined
Customs value (€)	0
Transport value (€)	0

FROM :
ESRF Magasin Tel: +33 (0)4 76 88 2733
6 rue Jules Horowitz +33 (0)4 76 88 2347
38042 Grenoble Fax: +33 (0)4 76 88 2347
FRANCE

1' For each component, print the labels by clicking on the printer icon
NB : This printer icon shows the attention sign until you have opened it once to print the labels

Once printed, stick label **1** and **2** to your dewar and box and put label **3** inside your dewar box for return (same action to do with any other shipment component like a backup in a box, a toolbox..)

How to: Track your shipment through ISPyB (first option)

► Shipment ► View ► Shipments

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

► Create

- Shipment
- Puck
- CSV upload

► View

- Shipments
- Dewars

Shipments													
Edit	Shipment Name	Creation date	Expected at ESRF	Sending details	Return details	# components (# samples)	View Dewars	View Samples	Comments	Status	History	Actions	
	demo	25-02-2014		MONACO-E.S.R.F.	MONACO-E.S.R.F.	1 (0)							
	ship1	25-02-2014		MONACO-E.S.R.F.	MONACO-E.S.R.F.	3 (0)							

Submit Shipping : demo

Creation date 2014-02-25 15:07:00.0

Courier company

Tracking number for Dewar1

Sending Date (DD-MM-YYYY)

Expected ESRF arrival date

Shipment status sent to ESRF

Warning: Once you've sent the shipment to The ESRF, you won't be able to modify the content of the shipment (dewars, containers, samples,...) and the information above. You will still be able to change sessions, add comments and modify Lab-Contacts.

Shipment Information

Dewar History

Dewar1 history view

Label

Dewar1

Barcode

ESRF0306349

Average customs values (Euro)

0

Average transport values (Euro)

0

Outbound courier

Outbound tracking number

Date	Status	Location
25-02-2014 15:13	ready to go	
25-02-2014 15:13	ready to go	
25-02-2014 15:37	sent to ESRF	

Return courier

Return tracking number

Shipment Information

Label

Number of

Creation date

Sending date

Expected date

Return date

Shipment Information		Dewar History	
Details			
Label	demo		
Number of components	1		
Creation date	25-02-2014		
Sending date	26-02-2014		
Expected arrival date	28-02-2014		
Return date			
Lab-contact for sending		Lab-contact for return	
Name	MONACO	Name	MONACO
Firstname	Stéphanie	Firstname	Stéphanie
Phone	33 (0)4 76 88 20 84	Phone	33 (0)4 76 88 20 84
Fax		Fax	
Email	monaco@esrf.fr	Email	monaco@esrf.fr
Lab name	E.S.R.F.	Lab name	E.S.R.F.
Lab address	6 rue Jules Horowitz B.P 220 F-38043 Grenoble Cedex France	Lab address	6 rue Jules Horowitz B.P 220 F-38043 Grenoble Cedex France

- 1 Send your shipment to ESRF
- 2 Fill in the details of the courier transport with your tracking number
- 3 View the history and the information of your shipment

How to: Track your shipment through ISPyB (second option)

► Shipment ► View ► Shipments

Lab-contacts

Shipment

Samples

Prepare experiment

Data collection

Feedback

References

Help

Log

► Create

Shipment

Puck

CSV upload

► View

Shipments








Dewars

Shipments

Edit	Shipment Name	Creation date	Expected at ESRF	Sending details	Return details	# components (# samples)	View Dewars	View Samples	Comments	Status	History	Actions
	demo	25-02-2014		MONACO-E.S.R.F.	MONACO-E.S.R.F.	1 (0)						
	ship1	25-02-2014		MONACO-E.S.R.F.	MONACO-E.S.R.F.	3 (0)						

All Components in Shipment : demo

Shipment comments :

Type	Comp. name	Comments	Barcode	Exp. date and beamline	tracking # TO Synchrotron	Tracking # FROM Synchrotron	Comp. status	ESRF Location	View Containers	View Samples	History	Comp. labels	Edit Comp. parameters	Other actions
	Dewar1		ESRF0306349	25/02/2014 ID23-2			sent to ESRF							

Dear User,

Your parcel Dewar1 (Proposal: FX##, Session date: 10-05-2013, Shipment: name date Barcode: ESRF #####) has been received by the ESRF on 06/05/2013 at 11:31 AM (GMT+0200) and will be dispatched to beamline:##

You can check its location at anytime via [ISPyB](#).

Don't hesitate to contact us at mxind@esrf.fr.

Best regards

The MXpress team

- 1 Click here to open bottom tab
- 2 Follow your shipment transport status
- 3 E-mail received when your components arrive on-site

How to: Describe the samples in your shipment

Procedure summary

This action requires steps 1 and 2 from the “How to ? : Track your shipment”

Option 1

On-line creation

- Fill in each puck of each dewar
- SAVE
- View all your samples in a list or per puck

Option 2

Excel upload

- Download your template filled with your protein acronyms
- Fill the template outside ISPyB
- Submit your .xls file

Option 3

CSV upload

- Prepare a file of the type on your computer
- Click on browse to select the file from your computer files
- Describe the field & text separator types
- Upload

How to:

Describe the samples of your shipment

On-line creation(1/2)

This action requires steps 1 and 2 from the “How to ? : Track your shipment”

Navigation menu: **Shipment** > **View** > **Shipments**

Lab contacts | **Shipment** | Samples | Prepare experiment | Data collection | Feedback | References | Help | Log out

Create

- Shipment
- Puck
- CSV upload

View

- Shipments**
- Dewars

Shipments												
Edit	Shipment Name	Creation date	Expected at ESRF	Sending details	Return details	# components (# samples)	View Dewars	View Samples	Comments	Status	History	Actions
	demo	25-02-2014	28-02-2014	MONACO-E.S.R.F.	MONACO-E.S.R.F.	1 (0)				sent to ESRF		
	ship1	25-02-2014				3 (0)						

Help

Dewar1 +

+

(*) mandatory field for each sample

1

2

- 1 You can directly access creation page via the View shipment page
- 2 Create the dewars and pucks you will need

How to: Describe the samples of your shipment *On-line creation(2/2)*

Help

Dewar1 +

Puck1 +

Save Reset Change sample name automatically

Sample Position	Protein Acronym (*)	Sample Name (*)	PinBarcode	Space Group	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	Comments
1	EP - Undefined			Un defi...				Default							
2								Default							
3								Default							
4								Default							
5								Default							
6								Default							
7								Default							
8								Default							
9								Default							
10								Default							

(*) mandatory field for each sample



Puck level
Each tab represents a puck.
Each row of the table represents a sample at a given position.
Sample names:
- Make sure the sample name contains only a-z, A-Z or 0-9 characters.
- Make sure the sample name is unique for a protein in the same dewar.
The experiment type should not be null, Default as default.

The top-left red icon in a cell indicates this field has been updated.

- + : to add a new puck to the selected dewar.
- ✓ : to change the selected puck label (to its barcode for example)
- 📄 : to copy a puck and its contents. You can then paste this in any other puck.
- 🗑️ : to copy the puck into the clipboard and remove it. You can then paste it in any other puck.
- 💾 : to save your modifications.
- ✗ : to remove this puck and its contents.
- ↺ : to reset the puck contents, all fields are set to their default values.
- ☒ Change sample name automatically : to automatically update the sample name with the increment number to the name of the 1st sample.

Experiment type definitions
These types are defined for automatic processes to be used in pilot studies. Don't use this field if you don't belong to a pilot study.
- manual = manual intervention by the crystallographer
- automatic = the sample is automatically prepared and diffracted

Shipment View Shipments

Lab-contactsShipmentSamplesPrepare experimentData collectionFeedbackReferencesHelp

Create

- Shipment
- Puck
- CSV upload

View

- Shipments
- Dewars

Shipments												
Edit	Shipment Name	Creation date	Expected at ESRF	Sending details	Return details	# components (# samples)	View Dewars	View Samples	Comments	Status	History	Actions
	demo	25-02-2014	28-02-2014	MONACO-E.S.R.F.	MONACO-E.S.R.F.	1 (0)				sent to ESRF		
	ship1	25-02-2014				3 (0)						

- 1 Fill in each puck of each dewar
- 2 SAVE (red corner = NOT saved)
- 3 Open help page if necessary



Export as PDF(sort by dewar/container/location)

Export as PDF(sort by acronym/sample name)

Samples

Protein	Space Group	Sample name	Smp code	Shipment	Dewar	Container	Loc. in cont.	Cell a	Cell b	Cell c	Cell alpha	Cell beta	Cell gamma	Crystal	Already observed	Required resol.	Minimal resol.	Sample comments	Edit sample	Sample status

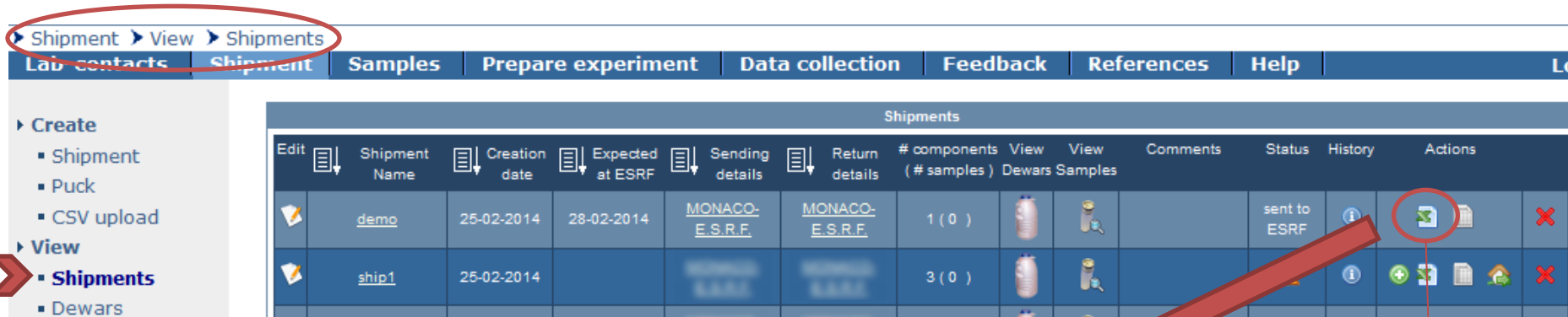
- 4 To view all your samples in a list or per puck and to export this list in pdf sorted by dewar/container/location or by acronym/sample name

How to:

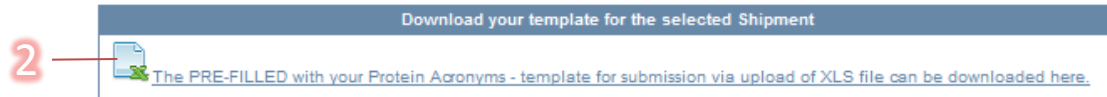
Describe the samples of your shipment

Excel Upload (1/2)

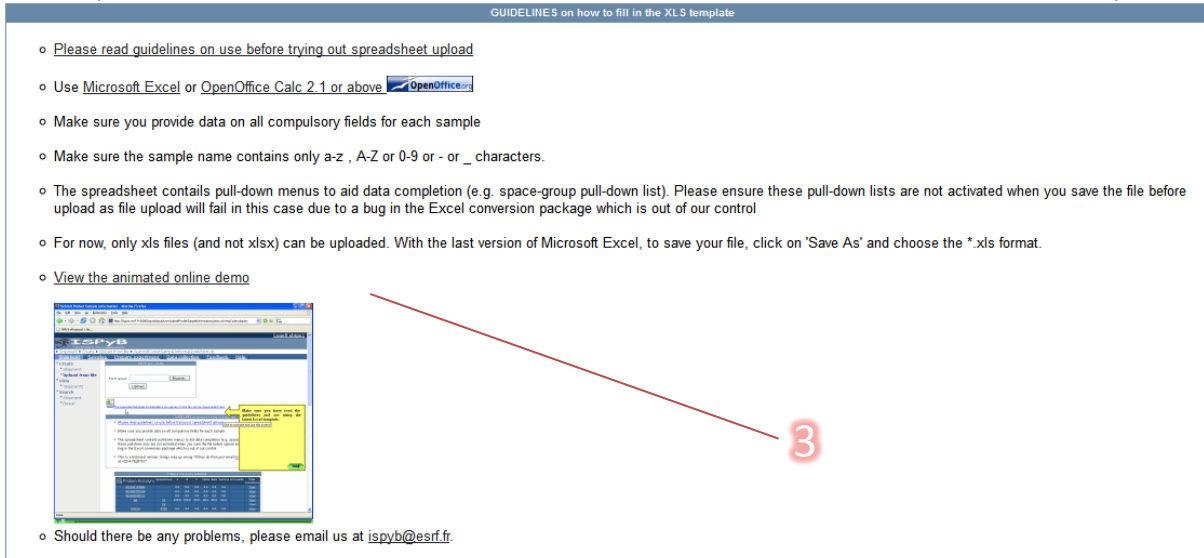
This action requires steps 1 and 2 from the “How to ? : Track your shipment”



The screenshot shows the ESFyB web interface. On the left, a sidebar menu has 'Shipments' highlighted under the 'View' section. The main content area is titled 'Shipments' and contains a table with columns: Edit, Shipment Name, Creation date, Expected at ESRF, Sending details, Return details, # components, View, View, Comments, Status, History, and Actions. Two shipments are listed: 'demo' and 'ship1'. In the 'Actions' column for the 'demo' shipment, an icon representing an Excel upload is circled in red and labeled with a red '1'. A large red arrow points from this icon towards the bottom right of the page.



This section is titled 'Download your template for the selected Shipment'. It contains a link: 'The PRE-FILLED with your Protein Acronyms - template for submission via upload of XLS file can be downloaded here.' A red '2' is placed next to a document icon on the left, with a red arrow pointing to the link.



This section is titled 'GUIDELINES on how to fill in the XLS template'. It contains several bullet points:

- Please read guidelines on use before trying out spreadsheet upload
- Use Microsoft Excel or OpenOffice Calc 2.1 or above
- Make sure you provide data on all compulsory fields for each sample
- Make sure the sample name contains only a-z, A-Z or 0-9 or - or _ characters.
- The spreadsheet contains pull-down menus to aid data completion (e.g. space-group pull-down list). Please ensure these pull-down lists are not activated when you save the file before upload as file upload will fail in this case due to a bug in the Excel conversion package which is out of our control
- For now, only xls files (and not xlsx) can be uploaded. With the last version of Microsoft Excel, to save your file, click on 'Save As' and choose the *.xls format.
- View the animated online demo

 At the bottom, there is a small screenshot of a video player showing an animated online demo, labeled with a red '3'. Below this, a red arrow points from the 'View the animated online demo' link to the video player. At the very bottom, there is a note: 'Should there be any problems, please email us at ispyb@esrf.fr'.

- 1 You can directly access the excel upload page via the View shipment page
- 2 Download your template filled with your protein acronyms
- 3 Use guidelines & videos at bottom of the page to fill the file

How to:

Describe the samples of your shipment

Excel Upload (2/2)

➤ Shipment ➤ View ➤ Shipments

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

➤ Create

- Shipment
- Puck
- CSV upload


➤ View

- Shipments**
- Dewars


➤ Search

- Shipment
- Dewar

Shipment
Name: demo
Creation date: 25-02-2014
Status: sent to ESRF
Back to this Shipment

 [Fill Shipment online](#)

Download your template for the selected Shipment

 [The PRE-FILLED with your Protein Acronyms - template for submission via upload of XLS file can be downloaded here.](#)

Submit your .xls file

The file must be a xls file (not.xlsx).

File to upload: No file selected.

Samples and Containers: ☐ Overwrite current shipment ☒ Add to current shipment

Warning :

"Overwrite current shipment" will delete the previously existing samples and pucks for that shipment.

"Add to current shipment" will add new pucks and samples to that shipment. Be aware that if a puck already exists with the same name or barcode it will be overwritten.

Please correct your file and re-submit it.

 [View Samples in Shipping](#)

- Cannot load file: [A-TIM + sampA1] is already exist unique. [A-TIM + sampA4] is already existing, and [A-TIM + sampA1] is already existing, and should be unique. [A-TIM + sampA4] is already existing, and should be unique.
- Warning: the unit cell parameters are not filled for the spaceGroup P2221 (A-TIM)!Warning: the unit cell parameters are not filled for the spaceGroup P2221 (A315S)!

Submit your .xls file :

- 1 Click on "Browse" to select the file on your computer
 - 2 Set the upload parameters: overwrite existing shipment content or add to current shipment
 - 3 Upload
 - 4 Example of error message that will appear if your file contains incorrect parameters
- NOTE : Make sure the uploaded file is of .xls format and not .xlsx format

How to: Describe the samples of your shipment *CSV Upload*

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample01	1		90	90	90	90	90	90
2	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample02	2		90	90	90	90	90	90
3	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample03	3		90	90	90	90	90	90
4	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample04	4		90	90	90	90	90	90
5	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample05	5		90	90	90	90	90	90
6	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample06	6		90	90	90	90	90	90
7	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	t2	thiolase	C222	0	sample07	7		90	90	90	90	90	90
8	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	CMY-10	beta-lactamase	P41212	0	sample08	8		90	90	90	90	90	90
9	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	CMY-10	beta-lactamase	P41212	0	sample09	9		90	90	90	90	90	90
10	mx	123	1	ship-20140214	Dewar1	Puck1	3	2.1	0.5	CMY-10	beta-lactamase	P41212	0	sample10	10		90	90	90	90	90	90
11	mx	123	1	ship-20140214	Dewar1	Puck2	3	2.1	0.5	t2	thiolase	C222	0	s01	1		90	90	90	90	90	90
12	mx	123	1	ship-20140214	Dewar1	Puck2	3	2.1	0.5	t2	thiolase	C222	0	s02	2		90	90	90	90	90	90
13	mx	123	1	ship-20140214	Dewar2	Puck3	3	2.1	0.5	t2	thiolase	C222	0	test01	1		90	90	90	90	90	90
14	mx	123	1	ship-20140214	Dewar2	Puck3	3	2.1	0.5	t2	thiolase	C222	0	test02	2		90	90	90	90	90	90

Shipment > Create > CSV upload

Lab-contacts Shipment Samples Prepare experiment Data

Create

- Shipment
- Puck
- CSV upload**

View

- Shipments
- Dewars

Search

- Shipment
- Dewar

Help

Submit your .csv file

The file must be a csv file.

File to upload

Browse...

No file selected.

Field separator

.

*

Text separator

,

*

Upload

- 1 Prepare a file of this type on your computer
- 2 Select the file from your computer files
- 3 Describe the field & text separator types
- 4 Upload

How to: Attach a new crystal form to a protein

► Samples ► Create ► New crystal form

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

► Create

- New sample
- **▪ New crystal form**

► View

- Proteins and crystal forms

► Search

- Protein
- Sample

► Update Database

Create a new Crystal Form

Please select a Protein Acronym **1**
this field is required

Geometry Class
Primitive triclinic
Primitive monoclinic
Centred monoclinic
Primitive orthorhombic
C-centred orthorhombic
I-centred orthorhombic
F-centred orthorhombic
Primitive tetragonal
I-centred tetragonal
Primitive trigonal
Primitive hexagonal
Rhombohedral
Primitive cubic
I-centred cubic
F-centred cubic
Rhombohedral hexagonal

Space Group

Morphology Color

Crystal size X Crystal size Y Crystal size Z

Comments

2

Go to Samples -> Create -> New crystal form

- 1** Choose your protein acronym (from the list populated with your sample sheets)
- 2** Enter the parameters of your new crystal form and save

How to: Upload a PDB file in view of automatic phasing (Dimple, autoMR, ...)

► Samples ► View ► Proteins and crystal forms

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

Click on the acronym, or on the space group to see the samples attached to corresponding acronym, space group.

Proteins and Crystal Forms List													
Protein Name	Protein Acronym	New Crystal SpaceGroup	A	B	C	Alpha	Beta	Gamma	Comments	Edit	Delete	PDB File	Data Collections
test	test1		108.668	180.159	101.144	90.0	110.3	90.0					View
test			32.016	33.281	48.002	77.97	70.54	61.28					View
Mnth	Mnth		R32	0.0	0.0	0.0	0.0	0.0					View
PA0688	PA0		P21	0.0	0.0	0.0	90.0	0.0	90.0				View

► Samples ► View ► Proteins and crystal forms

Lab-contacts Shipment Samples Prepare experiment

► Create
 ▪ New sample
 ▪ New crystal form
 ► View
 ▪ **Proteins and crystal forms**
 ► Search
 ▪ Protein
 ▪ Sample
 ► Update Database

Protein and Crystal Form

Acronym
[Back to this protein](#)

Space Group Undefined
[Back to this crystal form](#)

Uploaded Pdb

</data/pyapdb/mx415/4KMP.pdb>

Submit your pdb file

No file selected.

Update the unit cell parameters ☒

Go to Samples -> View -> Proteins and crystal forms

1 Click on "upload" (blue paper clip means that you already downloaded a PDB file for this protein/crystal)

2 Previously uploaded PDB file. Delete by clicking on the red cross. NB: If no PDB file has been previously uploaded there will be no box here.

3 Browse to select your PDB file and upload it. You can choose to update the unit cell parameters according to the data from the PDB file or not

How to: Search the database *Shipment/ Dewar and Data collection*

Shipment/ Dewar

1

Shipment

Lab-contacts Shipment Samples Prepare experiment Data collection

Create

- Shipment
- Puck
- CSV upload

View

- Shipments
- Dewars

Search

- Shipment
- Dewar

Search Shipping

Shipment label :

Creation date between DD-MM-YYYY :

and DD-MM-YYYY :

Reset Search

Search Dewars

Label

Comments

Experiment date between DD-MM-YYYY :

and DD-MM-YYYY :

Status

Location

Reset Search

5

Jul 2014

Sun	Mon	Tue	Wed	Thu	Fri	Sat
		1	2	3	4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30	31		

Data collection

3

Data collection

Lab-contacts Shipment Samples Prepare experiment Data collection

View last sessions

View all sessions

Search data collections

Search data collection

Sample name:

Protein acronym:

Beamline:

Experiment date between DD-MM-YYYY:

and DD-MM-YYYY:

Min number of images:

Max number of images:

Image prefix:

Max Data Collections retrieved:

Reset Search

4

You may use the * character to do a search with an incomplete Name.

Go to Shipment (1) or Data collection (2)

- 3 Click on Search -> "Shipment" (or "Dewar" or "data collections")
- 4 Fill in the parameters that you want to include in your search
- 5 If you want to search by date, click on the calendar icon and choose the date in the calendar
- 6 Click on "Search"

Tip: If you want to do a search with an incomplete name/label, use the * character

How to: Search the database *Protein/sample*

► Samples ► Search ► Protein

Lab-contacts | Shipment | **Samples** | Prepare

► Create

- New sample
- New crystal form

► View

- Proteins and crystal forms

► Search

- Protein
- Sample

Search Protein

Acronym

Reset Search

Go to Samples

- 1 Click on Search -> "Protein" (or "Sample")
- 2 Fill in the Protein Acronym, Sample name or Datamatrix Code
- 3 Click on "Search"

Tip: If you want to do a search with an incomplete name/label, use the * character

► Samples ► Search ► Sample

Lab-contacts | Shipment | **Samples** | Prepare exper

► Create

- New sample
- New crystal form

► View

- Proteins and crystal forms

► Search

- Protein
- **Sample**

Search Sample

Name

Datamatrix Code

Reset Search

How to: Populate your sample list in MXCuBE (sample changer content) with your samples described in ISPyB (1/2)

► Prepare experiment

Lab-contacts | Shipment | Samples | Prepare experiment | Data collection | Feedback | Referen

► Select Dewars

- Last dewars
- All dewars

► Fill sample changer

► View

- Selected dewars

Prepare your experiment:

1- Select the dewars you want for processing.
2- Fill the sample changer: assign a location for your containers
3- Associate data collections to samples in mxCuBE.

◀ ▶ First step: Select the dewars — 1

1 Select the Dewars → 2 Fill the Sample Changer → 3 Link Samples with Crystals

Prepare your experiment:

- 1- Select the dewar you want for processing.
- 2- Fill the sample changer: assign a location for your containers
- 3- In MxCuBe, link the samples in the container to the crystals in the Sample Changer.

◀ ▶ Next step: Fill the sample changer — 3

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

Select dewars for processing														
Ship. name	Creation date	Comp. name	Type	Comments	Barcode	Exp. date	Beamline	# containers (# samples)	Local contact	Dewar status	Location	View Containers	View Samples	Select for processing
test	07-07-2014	Dewar1			ESRF0308751			1 (3)		processing				Deselect
test	07-07-2014	test2		ghgdj	ESRF0308854			0 (0)		opened				Select
test	07-07-2014	Dewar1						0 (0)		opened				Select

Go to Prepare experiment

- 1 Click on "First step: Select the dewars"
- 2 Choose the dewar currently in use at the beamline
- 3 Click on "Next step: Fill the sample changer"

This action requires to have previously followed the
"How to ? : Track your shipment-> Create a shipment"

How to: Populate your sample list in MXCuBE with your samples described in ISPyB (2/2)

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.

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
test	07-07-2014	Dewar1	ESRF0306751	gdfdg	Puck	10	3		
ship-20140523	23-05-2014	Dewar1		Puck1	Puck	10	1	ID30A-1	1

Save

ESRF | EMBL | BM14 | SPINE | MSD | SO

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- 1 Choose the beamline and Sample changer location for each puck
- 2 Click on save
- 3 Log into mxCuBE
- 4 Click on "Synch ISPyB"

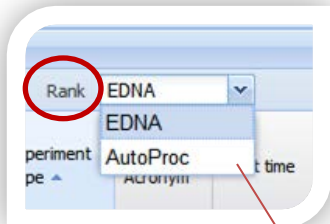
Prepare your experiment:

- 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.

The screenshot shows the mxCuBE interface with the 'Sample list' tab selected. The 'Sample list' shows a list of samples with columns for 'Sample', 'Mode', 'Centring', and 'Status'. The 'Sample' column lists various beamline locations (e.g., 1:1, 1:2, 1:3, 1:4, 1:5, 1:6, 1:7, 1:8, 1:9, 1:10, 2:1, 2:2, 2:3, 2:4). The 'Mode' column is set to 'Sample changer'. The 'Centring' column is set to 'Semi Automatic'. The 'Status' column shows 'Centring done' for the selected sample 1:5 - EL-te02.

The 'Synch ISPyB' button is highlighted with a red circle and labeled with a red '4'. The 'Sample list' is labeled with a red '3'.

How to: View all your processing results for a session & rank your samples



Search Sessions

Start Date	End Date	Beamline	Local contact	# Shifts	Comments	Edit	View session report	View collections groups	View collections
17-07-2014	18-07-2014	ID29		3	Session created by the BCM				
17-08-2014	18-08-2014	ID23-1		3	Session created by the BCM				
23-05-2014	24-05-2014	ID23-2		3	Session created by the BCM				
16-05-2014	17-05-2014	ID29		3	Session created by the BCM				

DataCollections

192 DataCollections

Save Experiment Parameters Rank EDNA

Image Prefix	Run No	Experiment Type	Protein Acronym	Start time	# images	Experiment Parameters	Status	Space Group	Completeness	Resolution	Rsymm Inner Outer Overall	Unit cell a, b, c alpha, beta, gamma	Sample Ranking	Skip
ref-centring_test_fine	4	Characteriz...		16-05-2014 11:09:23	4			P4		3.30		61.67, 61.67, 157.48 90.00, 90.00, 90.00	<input checked="" type="checkbox"/>	<input type="checkbox"/>
ref-centring_test	3	Characteriz...		16-05-2014 10:44:10	2			P4		2.82		61.66, 61.66, 157.49 90.00, 90.00, 90.00	<input checked="" type="checkbox"/>	<input type="checkbox"/>
ref-centring_test	2	Characteriz...		16-05-2014 10:42:48	2			P4		2.65		61.70, 61.70, 157.59 90.00, 90.00, 90.00	<input checked="" type="checkbox"/>	<input type="checkbox"/>

Go to Data collection

- 1 Click on "View collections"
- 2 Tick the "Sample Ranking" box of the samples that you want to rank
- 3 Select if you want to rank the results based on EDNA characterisation or autoprocessing results and click on "Rank"
- 4 View the ranking according to different parameters (clicking on the icon)

Tip: In the "view collection summary", sort the results by experiment type

Auto Proc Ranking (Rank - Value)

Select Sample	Image Prefix	Run No	Start time	Space Group	UC a	UC b	UC c	R-factor	Highest Resolution	Completeness	Total
<input checked="" type="checkbox"/>	CER-sampA01	1	12:29:08	P 41 21 2	62	62	159	#1 6.70	#1 1.94	#3 94.80	#1 94 %
<input checked="" type="checkbox"/>	CER-sampA02	1	12:37:37	P 41 21 2	62	62	159	#2 8.90	#2 2.01	#4 96.20	#2 84 %
<input checked="" type="checkbox"/>	CER-sampA04	1	12:57:16	P 41 21 2	62	62	159	#3 9.20	#3 2.13	#2 89.50	#3 83 %
<input checked="" type="checkbox"/>	CER-sampA03	1	12:45:21	P 41 21 2	62	62	159	#4 9.80	#4 2.16	#5 98.70	#4 79 %
<input checked="" type="checkbox"/>	centring_test_fine_w1	1	11:10:34	P 41 21 2	62	62	159	#5 17.90	#5 2.35	#1 76.90	#5 73 %

How to: View your experiment parameters and results

► Data collection

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

► View last sessions
► View all sessions
► Search data collections

Search Sessions

Last 20 sessions

Start Date	End Date	Beamline	Local contact	# Shifts	Comments	Edit	View session report	View collections groups	View collections	SMIS A-Form
17-07-2014	18-07-2014	ID29		3	Session created by the BCM					
17-06-2014	18-06-2014	ID23-1		3	Session created by the BCM					
23-05-2014	24-05-2014	ID23-2		3	Session created by the BCM					
16-05-2014	17-05-2014	ID29		3	Session created by the BCM					

Session

Save Comments | View All Summary info | View All DataCollection | Expand All | Collapse All | Clear Grouping

Experi- ment Type	Acronym Sample na	Image Pre	Run#	Parameters	Results	Image Thumbnail	Crystal snapshot	Graph	Second Graph	Comments
Start time: 12:57:16 16-05-2014 (1 Item)										
MXPres...	CER-sam pA04	CER-samp. 1		Nb tot images: 3817 Nb images: 3817 Exp. time: 0.04 s Phi range: 0.10 ° Flux: 1.69E11 ph/se Detector resolution: ... Transmission: 13.74 Wavelength: 0.976 Total expo time: 133...	MXPressE EDNA dp GrenADES fp GrenADES pp Space Group: P 41 21 2 Completeness:					

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

Go to Data collection

- 1 Click on "View session report" or on experiment date (1')
- 2 View the summary of your experiment parameters
- 3 Summary of the autoprocessing status and best results (cf p.58)
- 4 Summary snapshots and graphs for that experiment
- 5 Note that, by default, only the last 20 groups are displayed. Click here to access to the whole summary
- 6 Go to All data collection and access the downloadable autoprocessing files
- 7 Click on the Image prefix to access to experiment or beamline parameters and autoprocessing results for that experiment

How to: View/Download all autoprocessing files for one data collection

ment

Samples

Prepare experiment




















Data collection

Feedback

References

Search Sessions

Last 20 sessions

 Start Date	 End Date	 Beamline	Local contact	# Shifts	Comments	Edit	View session report	View collections groups	View collections	SMIS A-Form
17-07-2014	18-07-2014	ID29		3	Session created by the BCM					
17-06-2014	18-06-2014	ID23-1		3	Session created by the BCM					
23-05-2014	24-05-2014	ID23-2		3	Session created by the BCM					
16-05-2014	17-05-2014	ID29		3	Session created by the BCM					

1



2



DataCollections																
118 DataCollections																
Save	Experiment Parameters	Rank	EDNA													
Image Prefix	Run No	Experiment Type	Protein Acronym	Start time	# images	Experiment Parameters	Status	Space Group	Completeness	Resolution	Rsymm Inner Outer Overall	Unit_cell a, b, c alpha, beta, gamma	Sample Ranking	Skip	Comments	Download autoproc files
17-07-2014-01	1	OSC		20-07-2014 11:24:38	2240			P 1 21 1		49.11 - 6.7 1.79 - 1.73 49.11 - 1.73	2.2 123.8 5.2	87.71, 85.30, 150.30 90.00, 96.27, 90.00				
17-07-2014-02	1	OSC		20-07-2014 11:17:48	1414			P 1 21 1		49.76 - 7.05 1.88 - 1.82 49.76 - 1.82	4.6 479.1 40.3	87.65, 85.60, 150.20 90.00, 96.24, 90.00				
17-07-2014-03	2	OSC		20-07-2014 11:10:07	2250			P 1 21 1		49.34 - 7.32 1.96 - 1.89 49.34 - 1.89	3.4 5214.0 11.8	88.10, 85.84, 150.90 90.00, 96.23, 90.00				

Go to Data collection

1 Click on "View collections"

2 Click on the green arrow to download all Autoprocessing files at once

How to: View/Download specific autoprocessing results

Experiment Samples Prepare experiment **Data collection** Feedback References

Search Sessions

Last 20 sessions									
Start Date	End Date	Beamline	Local contact	# Shifts	Comments	Edit	View session report	View collections groups	View collections
17-07-2014	18-07-2014	ID29		3	Session created by the BCM				
17-06-2014	18-06-2014	ID23-1		3	Session created by the BCM				
23-05-2014	24-05-2014	ID23-2		3	Session created by the BCM				
16-05-2014	17-05-2014	ID29		3	Session created by the BCM				

Session

Save Comments View All DataCollection

Experiment Type	Acronym Sample na	Image Pre	Run#	Parameters	Results	Image Thumbnail
MXPres...	CER-san pA04	CER-samp, 1		Nb tot images: 3817 Nb images: 3817 Exp. time: 0.04 s Phi range: 0.10 ° Flux: 1.69E11 ph/se Detector resolution: ... Transmission: 13.74 Wavelength: 0.976 Total expo time: 133...	MXPressE EDNA dp GrenADES fp GrenADES pp Space Group: P 41 21 2 Completeness:	

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)							
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
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: Update

View Data Collection Statistics:

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 °

Files

Download

XDS XSCALE SCALE/AINLESS SCALEPACK TRUNCATE

Input Files:

scala_noanom.inp

Log Files:

merged_noanom_XSCALE.LP

Go to Data collection

- 1 Click on "View session report"
- 2 Click on the Image prefix then go to the AutoProcessing tab
- 3 Select the autoprocessing result you want to view in particular
- 4 Click on the file name to view a file or on the green arrow to download all the files for that autoprocessing at once
- 5 View the statistics report for this data collection
- 6 Click on the graph icon to view graph extracted from the corresponding log file

How to: View your processing results -EDNA characterisation

► Data collection

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

► View last sessions
► View all sessions
► Search data collections

Search Sessions

Last 20 sessions

Start Date	End Date	Beamline	Local contact	# Shifts	Comments	Edit	View session report	View collections groups	View collections	SMIS A-Form
17-07-2014	18-07-2014	ID29		3	Session created by the BCM					
17-06-2014	18-06-2014	ID23-1		3	Session created by the BCM					
23-05-2014	24-05-2014	ID23-2		3	Session created by the BCM					
16-05-2014	17-05-2014	ID29		3	Experiment test: data starting on 16 and 17 sep 2014					

Session

Save Comments View All DataCollection

Experiment Type	Acronym Sample name	Image Prefix	Run#	Parameters	Results
Start time: 11:09:23 16-05-2014 (1 Item)					
Characterization	ref-centring_test_fine_4			Nb images: 4 Exp. time: 0.20 s Phi range: 1.00 ° Flux: 3.63E11 ph/sec Detector resolution: 2.00 Å Transmission: 100.00 Wavelength: 0.976 Å Total expo time:	Indexing Strategy Space Group: P4 Unit Cell: a, b, c: 61.67, 61.67, 157.48 α, β, γ: 90.00, 90.00, 90.00 Mosaicity: 0.38 Å Ranking Resolution: 3.30 Å

Experiment parameters Beamline parameters Characterisation parameters **Characterisation results** AutoProcessing

Characterisation Results ([EDNA log file](#))

Data collection info

Data collection date	2014/May/16 11:09:35.889
Image prefix	ref-centring_test_fine_4

Go to Data collection

- 1 Click on "View session report"
- 2 Click on the Image prefix then go to the "Characterisation results" tab to obtain more details

How to: Extract reports

► Data collection

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

View last sessions
View all sessions
Search data collections

Search Sessions

Start Date	End Date	Beamline	Local contact	# Shifts	Comments	Edit	View session report	View collections groups	View collections	SMIS A-Form
17-07-2014	18-07-2014	ID29		3	Session created by the BCM					
17-06-2014	18-06-2014	ID23-1		3	Session created by the BCM					
23-05-2014	24-05-2014	ID23-2		3	Session created by the BCM					
16-05-2014	17-05-2014	ID29		3	MXpressOE tests: New setting on A2 and SA test results					



► Data collection

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

View last sessions
View all sessions
Search data collections

Selected Session

Start Date: 16-05-2014
BeamLine: ID29 +33476882805
[Back to this session](#)
[Back to sessions](#)

Session Information

Local Contact:
Comments: MXpressOE tests: New setting on A2 and SA test results

Session Statistics

Nb Collect:	179
Nb Test:	13
Nb Energy Scan:	0
Nb XRFspectra:	0

Reports

General report:
Screening report:
MXPressO-MXPressE report:

Go to Data collection

- 1 Click on View session report
- 2 Click on the icon to download the report either in word or PDF format