

How to ?

=> Use the new shipment/sample form in ISPyB

Create a Lab-contact

=> If your lab-contact already exists please go directly to next page

Lab-contacts > Create > LabContact

Lab-contacts | Shipment | Samples | Prepare experiment

Create

- LabContact

View

- LabContacts

New/Edit LabContact

Scientist name

Scientist firstname

Search contact

• No match found in SMIS Database.

New/Edit LabContact

Scientist name

Scientist firstname

Search contact

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)

Save card

- 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 ?

=> Use the new
shipment/sample form in ISPyB

Create a Shipment

Shipment > Create > Shipment

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

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 address (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 & 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 ?

=> Use the new
shipment/sample form in ISPyB

Describe the samples of my shipment

To use it during my experiment at the beamline

Option 1

On-line creation

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

Option 2

Excel upload

- Download your template filled with your protein acronyms
- Fill the template
- 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 sample of my shipment

Option 1 : On-line creation (1/2)

This action requires the lab-contact creation and shipment creation steps (see previously).

- 1 If this was previously done, directly access the creation page via the View shipment page
- 2 Create the dewars and pucks you will need

Navigation: Shipment > View > Shipments

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

Create

- Shipment
- Puck
- CSV upload

View

- Shipments**
- Dewars

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		MONACO-E.S.R.F.	MONACO-E.S.R.F.	3 (0)						

2

Help

Dewar1 +

+

(*) mandatory field for each sample

1

How to ?

=> Describe the sample of my shipment

Option 1 : 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

Remove the selected dewar and its contents.

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 experiment.
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 increment number to the name of the 1st sample.

Experiment type definitions
These types are defined for automatic processes to perform. Don't use this field if you don't belong to a specific group.
Manual = manual intervention by the crystallographer.
Automatic = the sample is automatically processed.

Shipment View Shipments

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

Create

- Shipment
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View

- Shipments
- Dewars

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)						

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

Export as PDF (sort by acronym/sample name)

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

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