

How to ?

=> Describe the samples of my shipment

To use it during my experiment at the beamline

Procedure summary :

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

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 steps 1 and 2 from the “How to ? : Track my shipment”

1 If this was previously done, directly access creation page via the View shipment page

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)						

Help

Dewar1 +

+

(*) mandatory field for each sample

2 Create the dewars and pucks you will need

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 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 this 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 data collection. 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 prepared and data collection is performed.

Shipment View Shipments

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

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	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)

4

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 sample of my shipment

Option 2 : Excel upload (1/2)

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

1 If this was previously done, directly access excel upload page via the View shipment page

Shipments

Edit	Shipment Name	Creation date	Expected at ESRF	Sending details	Return details	# components (# samples)	Dewars	View	View	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)							

2

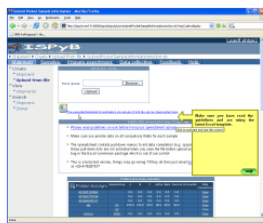
Download your template for the selected Shipment

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

GUIDELINES on how to fill in the XLS template

- 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](#)

3



- Should there be any problems, please email us at ispyb@esrf.fr.

- 2 Download your template filled with your protein acronyms
- 3 Use guidelines & videos at bottom of page to fill the file

How to ?

=> Describe the sample of my shipment

Option 2 : 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.

Submit your .xls file :

- 1 Select from your computer (browse)
- 2 Select to overwrite existing shipment content or to add to current shipment
- 3 Upload

NOTE : Make sure it is of .xls format and not .xlsx format

How to ?

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Option 3 : 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 the type on your computer
- 2 Select the file from your computer files
- 3 Describe the field & text separator types
- 4 Upload