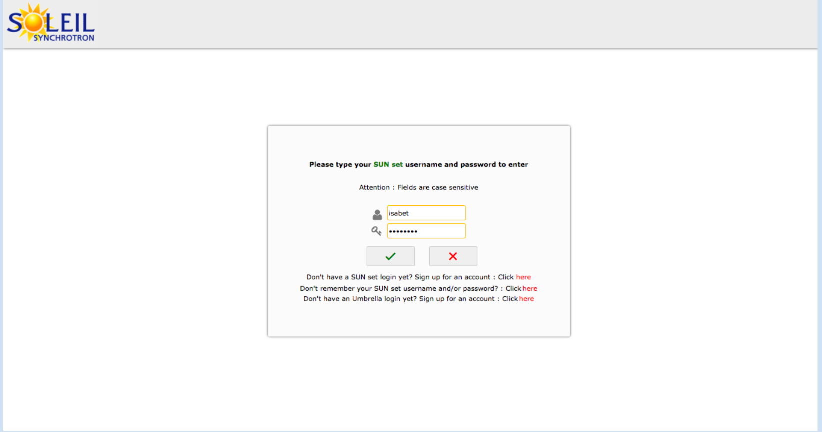
ISPyB manual

Connection via SunSET

Login in the SunSET



Please type your SUN set username and password to enter

Attention : Fields are case sensitive

isabet

••••••••

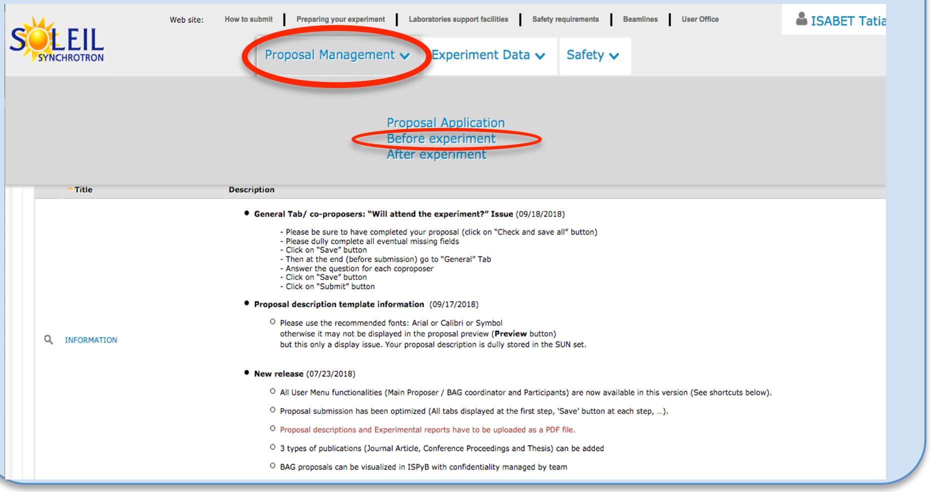
✓ ✗

Don't have a SUN set login yet? Sign up for an account : Click here

Don't remember your SUN set username and/or password? : Click here

Don't have an Umbrella login yet? Sign up for an account : Click here

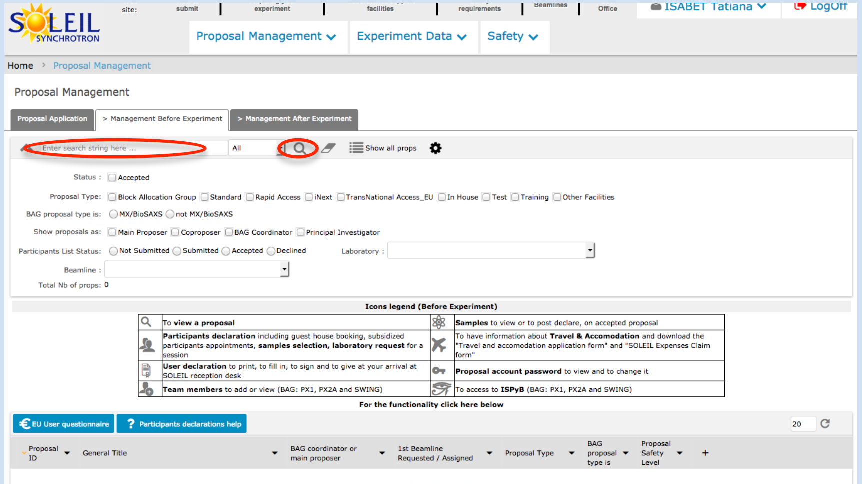
Search for your project-1



- **General Tab/ co-proposers: "Will attend the experiment?" Issue** (09/18/2018)
  - Please be sure to have completed your proposal (click on "Check and save all" button)
  - Please dully complete all eventual missing fields
  - Click on "Save" button
  - Then at the end (before submission) go to "General" Tab
  - Answer the question for each coproposer
  - Click on "Save" button
  - Click on "Submit" button
- **Proposal description template information** (09/17/2018)
  - Please use the recommended fonts: Arial or Calibri or Symbol
    otherwise it may not be displayed in the proposal preview (**Preview** button)
    but this only a display issue. Your proposal description is dully stored in the SUN set.
- **New release** (07/23/2018)
  - All User Menu functionalities (Main Proposer / BAG coordinator and Participants) are now available in this version (See shortcuts below).
  - Proposal submission has been optimized (All tabs displayed at the first step, 'Save' button at each step, …).
  - Proposal descriptions and Experimental reports have to be uploaded as a PDF file.
  - 3 types of publications (Journal Article, Conference Proceedings and Thesis) can be added
  - BAG proposals can be visualized in ISPyB with confidentiality managed by team

Search for your project-2

Enter your project number and then click on the magnifying loop



Status : ☐ Accepted

Proposal Type: ☐ Block Allocation Group ☐ Standard ☐ Rapid Access ☐ iNext ☐ TransNational Access_EU ☐ In House ☐ Test ☐ Training ☐ Other Facilities

BAG proposal type is: ○ MX/BioSAXS ○ not MX/BioSAXS

Show proposals as: ☐ Main Proposer ☐ Coproposer ☐ BAG Coordinator ☐ Principal Investigator

Participants List Status: ○ Not Submitted ○ Submitted ○ Accepted ○ Declined

Laboratory :

Beamline :

Total Nb of props: 0

Icons legend (Before Experiment)

🔍	To **view a proposal**		**Samples** to view or to post declare, on accepted proposal
	Participants declaration including guest house booking, subsidized participants appointments, **samples selection, laboratory request** for a session	✈	To have information about **Travel & Accomodation** and download the "Travel and accomodation application form" and "SOLEIL Expenses Claim form"
	User declaration to print, to fill in, to sign and to give at your arrival at SOLEIL reception desk		**Proposal account password** to view and to change it
	Team members to add or view (BAG: PX1, PX2A and SWING)		To access to **ISPyB** (BAG: PX1, PX2A and SWING)

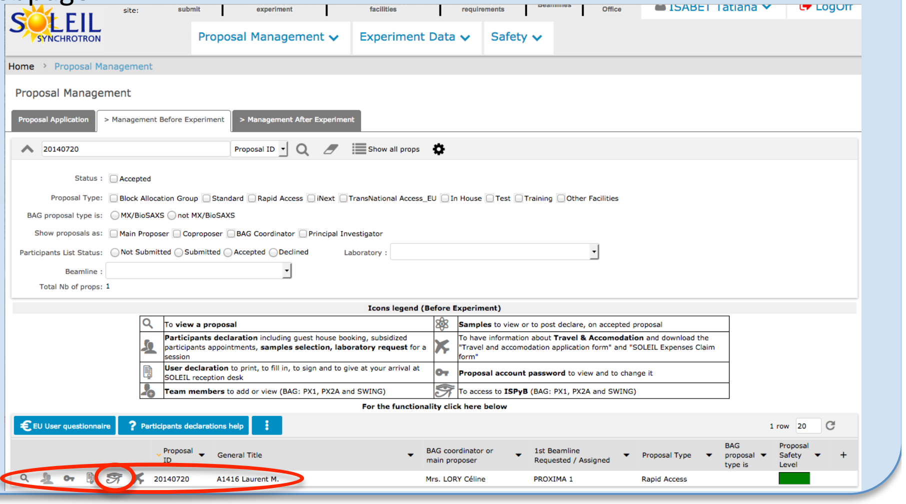
For the functionality click here below

Proposal ID	General Title	BAG coordinator or main proposer	1st Beamline Requested / Assigned	Proposal Type	BAG proposal type is	Proposal Safety Level

No results have been loaded yet.

Project appears at the bottom with the ISPyB icon

Click on the Eye icon, a new tab window will be opened with ISPyB webpage



20140720

Status : ☐ Accepted

Proposal Type: ☐ Block Allocation Group ☐ Standard ☐ Rapid Access ☐ iNext ☐ TransNational Access_EU ☐ In House ☐ Test ☐ Training ☐ Other Facilities

BAG proposal type is: ○ MX/BioSAXS ○ not MX/BioSAXS

Show proposals as: ☐ Main Proposer ☐ Coproposer ☐ BAG Coordinator ☐ Principal Investigator

Participants List Status: ○ Not Submitted ○ Submitted ○ Accepted ○ Declined

Laboratory :

Beamline :

Total Nb of props: 1

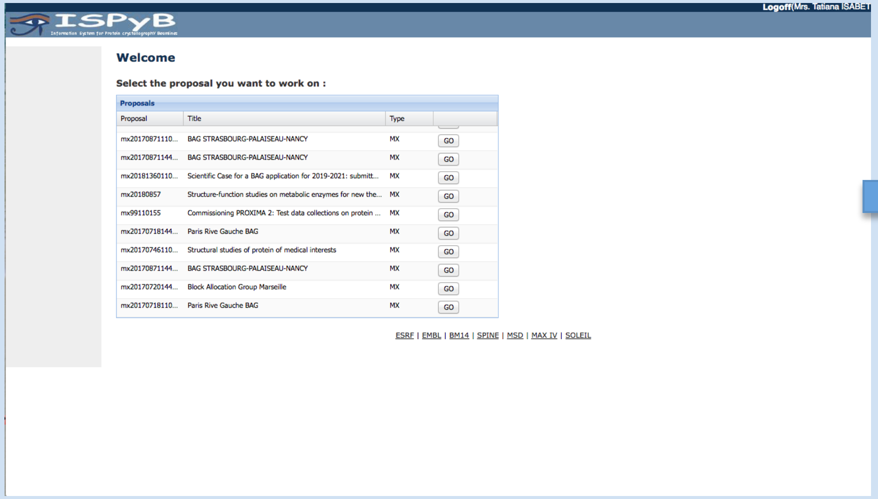
Icons legend (Before Experiment)

🔍	To **view a proposal**		**Samples** to view or to post declare, on accepted proposal
	Participants declaration including guest house booking, subsidized participants appointments, **samples selection, laboratory request** for a session	✈	To have information about **Travel & Accomodation** and download the "Travel and accomodation application form" and "SOLEIL Expenses Claim form"
	User declaration to print, to fill in, to sign and to give at your arrival at SOLEIL reception desk		**Proposal account password** to view and to change it
	Team members to add or view (BAG: PX1, PX2A and SWING)		To access to **ISPyB** (BAG: PX1, PX2A and SWING)

For the functionality click here below

Proposal ID	General Title	BAG coordinator or main proposer	1st Beamline Requested / Assigned	Proposal Type	BAG proposal type is	Proposal Safety Level
20140720	A1416 Laurent M.	Mrs. LORY Céline	PROXIMA 1	Rapid Access		🟩

Click GO on the right project



Welcome

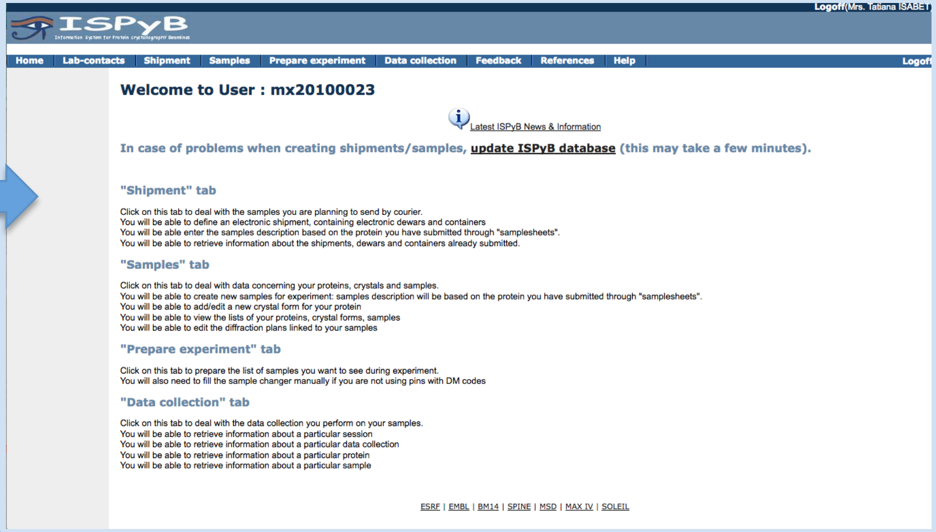
Select the proposal you want to work on :

Proposals

Proposal	Title	Type	
mx20170871110...	BAG STRASBOURG-PALAISEAU-NANCY	MX	GO
mx20170871144...	BAG STRASBOURG-PALAISEAU-NANCY	MX	GO
mx20181360110...	Scientific Case for a BAG application for 2019-2021: submitt...	MX	GO
mx20180857	Structure-function studies on metabolic enzymes for new the...	MX	GO
mx99110155	Commissioning PROXIMA 2: Test data collections on protein ...	MX	GO
mx20170718144...	Paris Rive Gauche BAG	MX	GO
mx20170746110...	Structural studies of protein of medical interests	MX	GO
mx20170871144...	BAG STRASBOURG-PALAISEAU-NANCY	MX	GO
mx20170720144...	Block Allocation Group Marseille	MX	GO
mx20170718110...	Paris Rive Gauche BAG	MX	GO

ESRF | EMBL | BM14 | SPINE | MSD | MAX IV | SOLEIL

ISPyB Mainpage



Welcome to User : mx20100023

Latest ISPyB News & Information

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 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

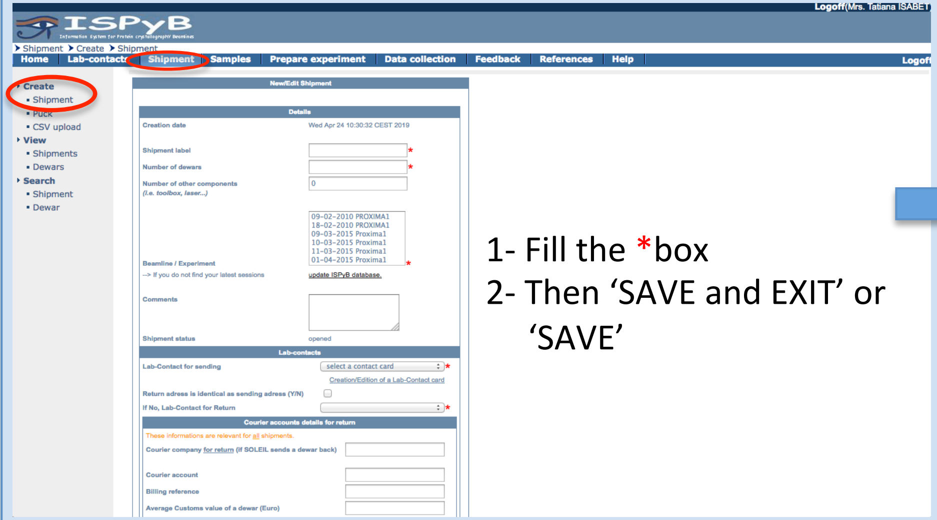
Click on this tab to prepare the list of samples you want to see during experiment.
You will also need to fill the sample changer manually if you are not using pins with DM codes

"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 | EMBL | BM14 | SPINE | MSD | MAX IV | SOLEIL

1- Create a shipment



New/Edit Shipment

Details

Creation date: Wed Apr 24 10:30:32 CEST 2019
Shipment label: *
Number of dewars: *
Number of other components (i.e. toolbox, laser...): 0
Beamline / Experiment: 09-02-2010 PROXIMA1, 18-02-2010 PROXIMA1, 09-03-2015 Proxima1, 10-03-2015 Proxima1, 11-03-2015 Proxima1, 01-04-2015 Proxima1 *
--> If you do not find your latest sessions: update ISPyB database.
Comments:
Shipment status: opened

Lab-contacts

Lab-Contact for sending: select a contact card *
Creation/Edition of a Lab-Contact card
Return adress is identical as sending adress (Y/N) ☐
If No, Lab-Contact for Return: *

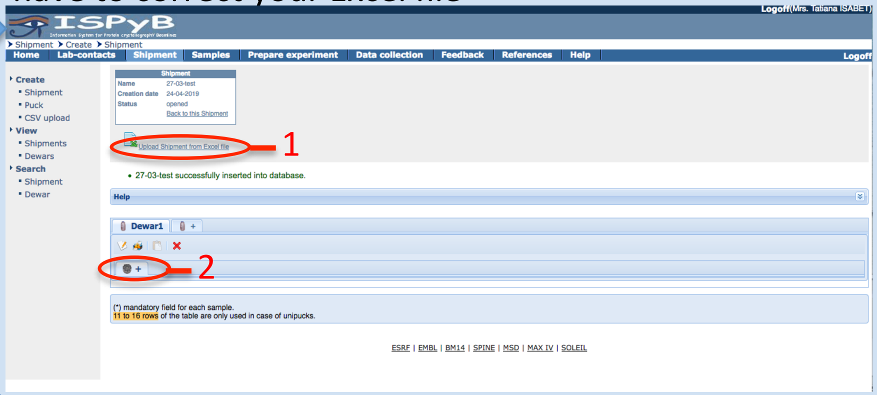
Courier accounts details for return

These informations are relevant for all shipments.
Courier company for return (if SOLEIL sends a dewar back):
Courier account:
Billing reference:
Average Customs value of a dewar (Euro):

1- Fill the *box
2- Then ‘SAVE and EXIT’ or ‘SAVE’

2- Upload your Excel file (1) or add components by hand (2)

In the case of Excel upload, after uploading, all the messages should appear in Green. If you see Red messages, it means something went wrong, and you will have to correct your Excel file



Shipment

Name	27-03-test
Creation date	24-04-2019
Status	opened
	Back to this Shipment

- 27-03-test successfully inserted into database.

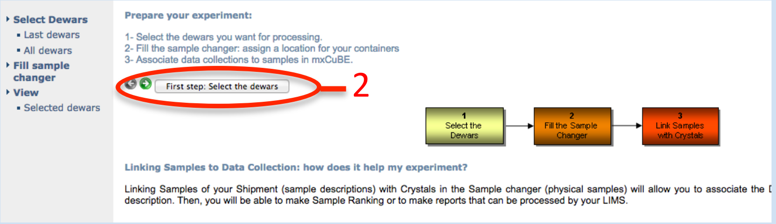
(*) mandatory field for each sample.
11 to 16 rows of the table are only used in case of unipucks.

ESRF | EMBL | BM14 | SPINE | MSD | MAX IV | SOLEIL

3- Prepare your experiment

1- Click on ‘Prepare experiment’ on the top menu

2- Click on First step : Select the dewars



Prepare your experiment:

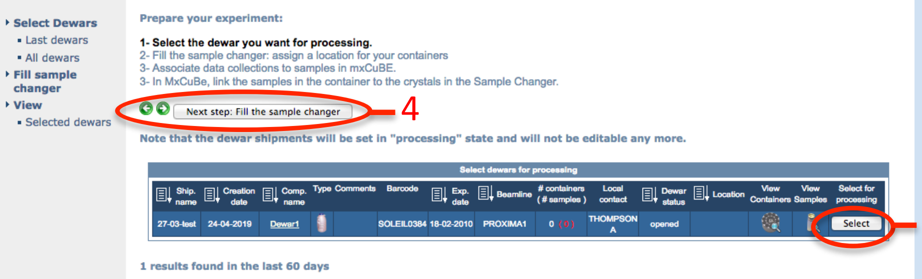
1- Select the dewars you want for processing.
2- Fill the sample changer: assign a location for your containers
3- Associate data collections to samples in mxCuBE.

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
description. Then, you will be able to make Sample Ranking or to make reports that can be processed by your LIMS.

3- Select the proper session (appear in orange background)

4- Then click on Next step : Fill the sample changer



Prepare your experiment:

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

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

Select dewars for processing

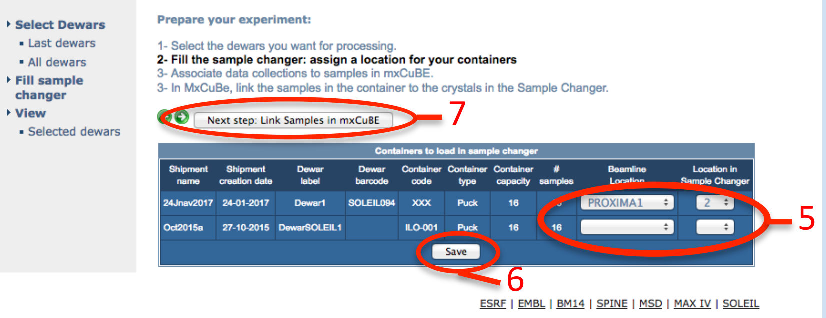
Ship. name	Creation date	Comp. name	Type	Comments	Barcode	Exp. date	Beamline	# containers (# samples)	Local contact	Dewar status	Location	View Containers	View Samples	Select for processing
27-03-test	24-04-2019	Dewar1			SOLEIL0384	18-02-2010	PROXIMA1	0 (0)	THOMPSON A	opened				Select

1 results found in the last 60 days

5- Select the beamline and the puck location

6- Don’t forget to SAVE (it takes some seconds)

7- Then click on Next step : Link Samples in MXCuBE



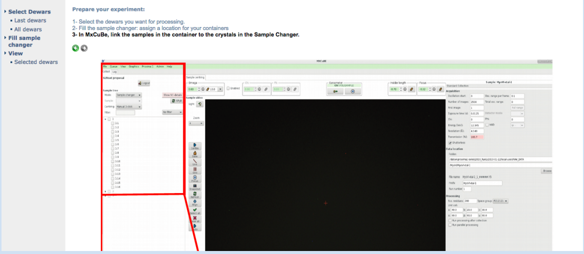
Prepare your experiment:

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

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
24Jnav2017	24-01-2017	Dewar1	SOLEIL094	XXX	Puck	16	[illegible]	PROXIMA1	2
Oct2015a	27-10-2015	DewarSOLEIL1		ILO-001	Puck	16	16		

Final page : if you arrived here, it means that you can click on the ISPyB synchronisation button within MXCuBE



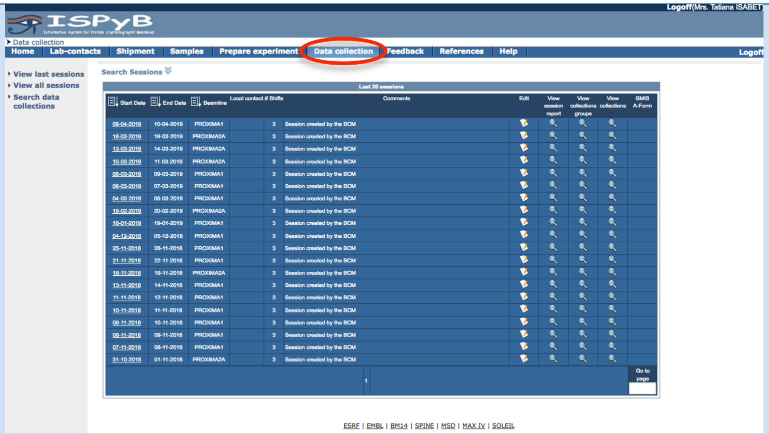
Prepare your experiment:

1- Select the dewars 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.

4- Data collection

1- Click on Data collection on the top menu

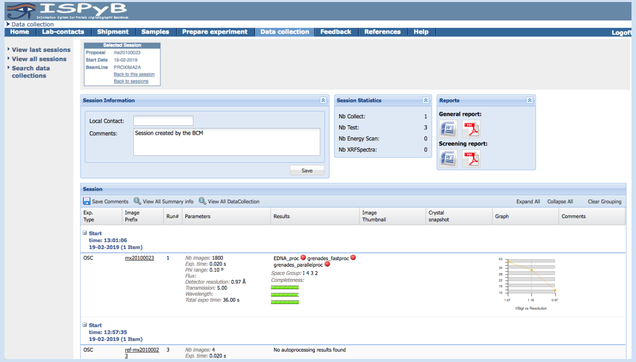
2- Click on your session



Last 20 sessions

Start Date	End Date	Beamline	Local contact	# Shifts	Comments	Edit	View session report	View collections groups	View collections	SMIS A-Form
09-04-2019	10-04-2019	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
18-03-2019	19-03-2019	PROXIMA2A		3	Session created by the BCM	✎	🔍	🔍	🔍	
13-03-2019	14-03-2019	PROXIMA2A		3	Session created by the BCM	✎	🔍	🔍	🔍	
10-03-2019	11-03-2019	PROXIMA2A		3	Session created by the BCM	✎	🔍	🔍	🔍	
08-03-2019	09-03-2019	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
06-03-2019	07-03-2019	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
04-03-2019	05-03-2019	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
19-02-2019	20-02-2019	PROXIMA2A		3	Session created by the BCM	✎	🔍	🔍	🔍	
18-01-2019	19-01-2019	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
04-12-2018	05-12-2018	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
25-11-2018	26-11-2018	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
21-11-2018	22-11-2018	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
18-11-2018	19-11-2018	PROXIMA2A		3	Session created by the BCM	✎	🔍	🔍	🔍	
13-11-2018	14-11-2018	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
11-11-2018	12-11-2018	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
10-11-2018	11-11-2018	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
09-11-2018	10-11-2018	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
08-11-2018	09-11-2018	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
07-11-2018	08-11-2018	PROXIMA1		3	Session created by the BCM	✎	🔍	🔍	🔍	
31-10-2018	01-11-2018	PROXIMA2A		3	Session created by the BCM	✎	🔍	🔍	🔍	

A list of data collection appears with results of autoprocessing



Selected Session
Proposal mx20100023
Start Date 19-02-2019
BeamLine PROXIMA2A

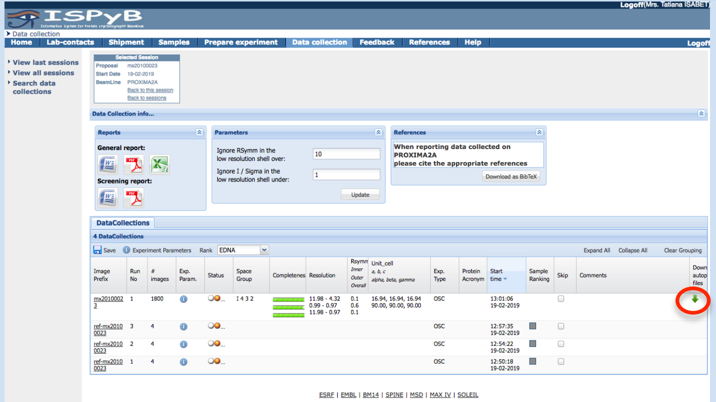
Local Contact:
Comments: Session created by the BCM

Nb Collect: 1
Nb Test: 3
Nb Energy Scan: 0
Nb XRFSpectra: 0

Exp. Type	Image Prefix	Run#	Parameters	Results	Image Thumbnail	Crystal snapshot	Graph	Comments
Start time: 13:01:06 19-02-2019 (1 Item)								
OSC	mx20100023	1	Nb images: 1800 Exp. time: 0.020 s Phi range: 0.10 ° Flux: Detector resolution: 0.97 Å Transmission: 5.00 Wavelength: Total expo time: 36.00 s	EDNA_proc ● grenades_fastproc ● grenades_parallelproc ● Space Group: I 4 3 2 Completeness:				
Start time: 12:57:35 19-02-2019 (1 Item)								
OSC	ref-mx20100023	3	Nb images: 4 Exp. time: 0.020 s	No autoprocessing results found				

If you click on **View All DataCollection**, a new display appears : you can see results with a different graphical display in which you can download results (mtz file and logs)

If you click on a data collection, you will find more autoprocessing detailed results



Selected Session
Proposal mx20100023
Start Date 19-02-2019
BeamLine PROXIMA2A

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

When reporting data collected on PROXIMA2A please cite the appropriate references

4 DataCollections

Rank EDNA

Image Prefix	Run No	# images	Exp. Param.	Status	Space Group	Completeness	Resolution	Rsymm Inner Outer Overall	Unit_cell a, b, c alpha, beta, gamma	Exp. Type	Protein Acronym	Start time	Sample Ranking	Skip	Comments	Down autop files
mx20100023	1	1800	ⓘ	○●...	I 4 3 2		11.98 - 4.32 0.99 - 0.97 11.98 - 0.97	0.1 0.6 0.1	16.94, 16.94, 16.94 90.00, 90.00, 90.00	OSC		13:01:06 19-02-2019		☐		↓
ref-mx20100023	3	4	ⓘ	○●...						OSC		12:57:35 19-02-2019	■	☐		
ref-mx20100023	2	4	ⓘ	○●...						OSC		12:54:22 19-02-2019	■	☐		
ref-mx20100023	1	4	ⓘ	○●...						OSC		12:50:18 19-02-2019	■	☐		