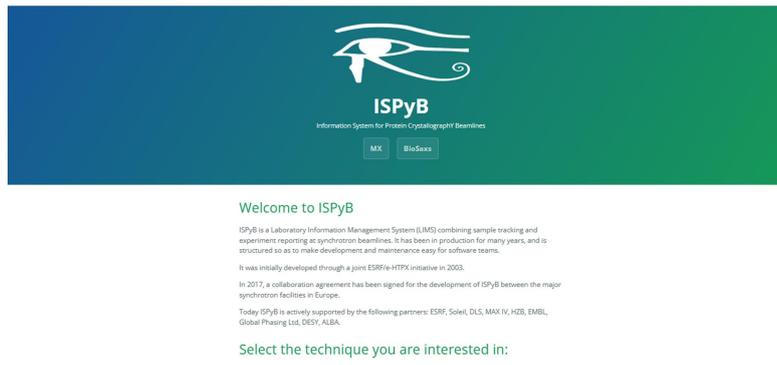


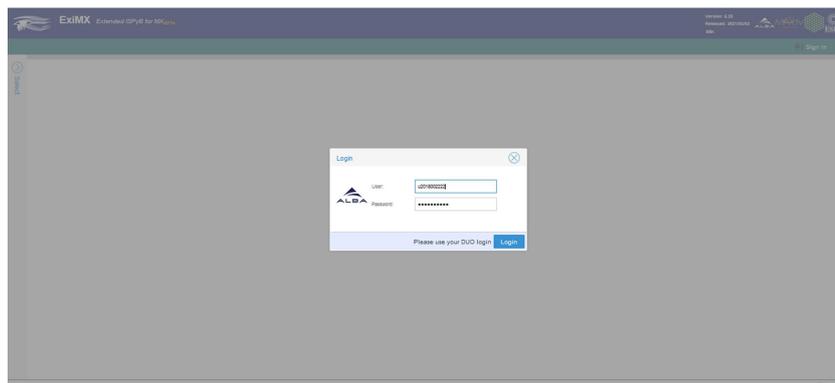
ISPyB EXI User Manual XALOC Beamline

HOW TO SEND YOUR DEWARS TO ALBA

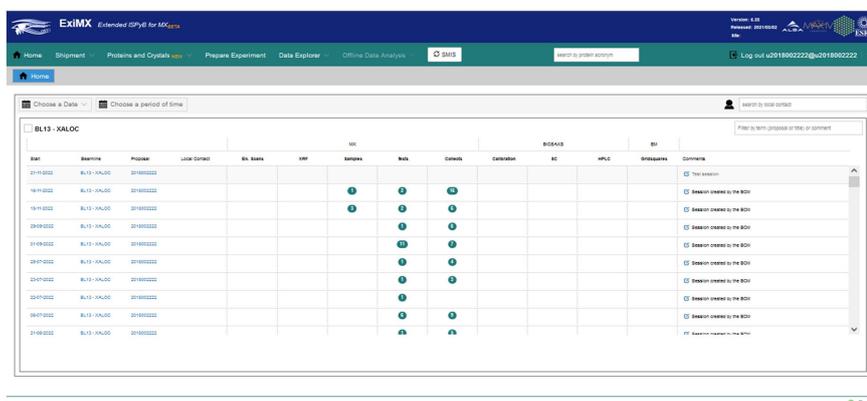
- In your favourite web browser go to <https://ispyb.cells.es/> and choose MX (Fig 1).



- **Login to EXI** using the credentials of your proposal (u202xxxxxxx) (Fig. 2).

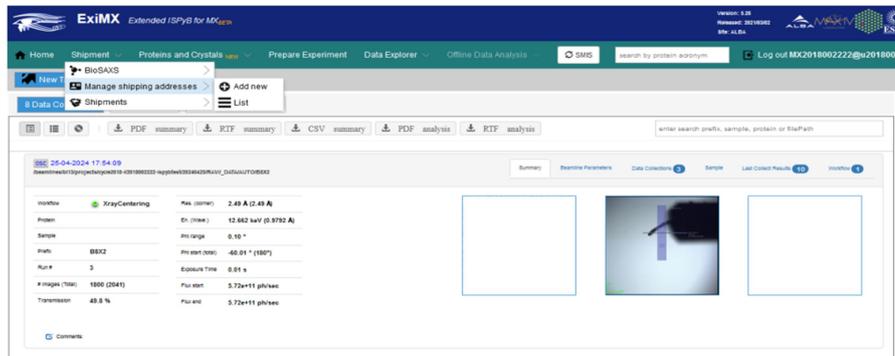


- In order to load your samples in EXI, first **click on the session** corresponding to your beamtime (in the example shown, 21/11/2022) (Fig. 3)

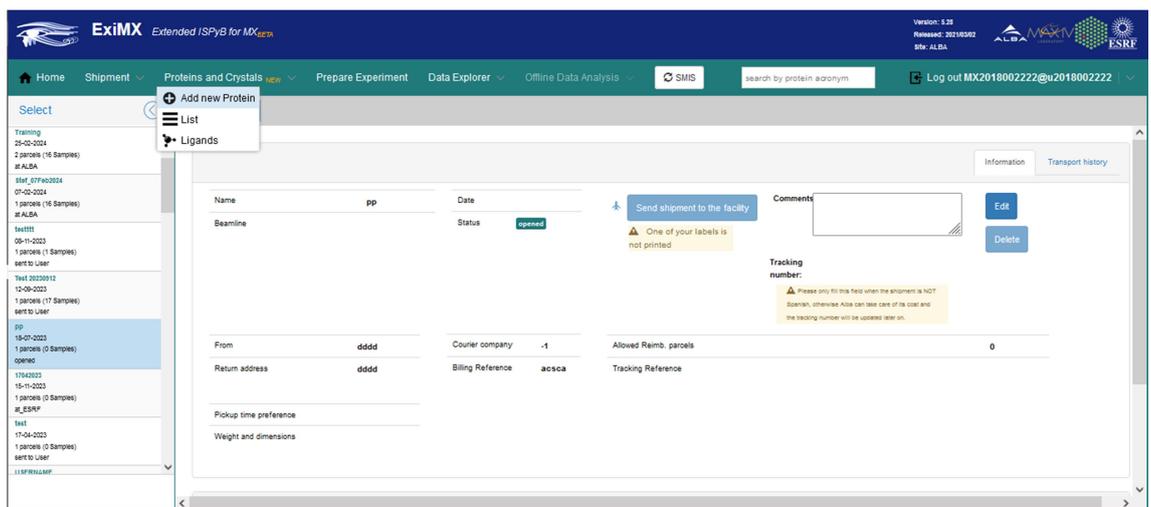


Date	Beamtime	Proposal	User	Status	Technical Parameters
21/11/2022	BL13-XALOC	2018000222		1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100
18/11/2022	BL13-XALOC	2018000222		1	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, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100
19/11/2022	BL13-XALOC	2018000222		1	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, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100
20/11/2022	BL13-XALOC	2018000222		1	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, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100
01/10/2022	BL13-XALOC	2018000222		1	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, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100
20/11/2022	BL13-XALOC	2018000222		1	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, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100
20/11/2022	BL13-XALOC	2018000222		1	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, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100
20/11/2022	BL13-XALOC	2018000222		1	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, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100
20/11/2022	BL13-XALOC	2018000222		1	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, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100
21/11/2022	BL13-XALOC	2018000222		1	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, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100

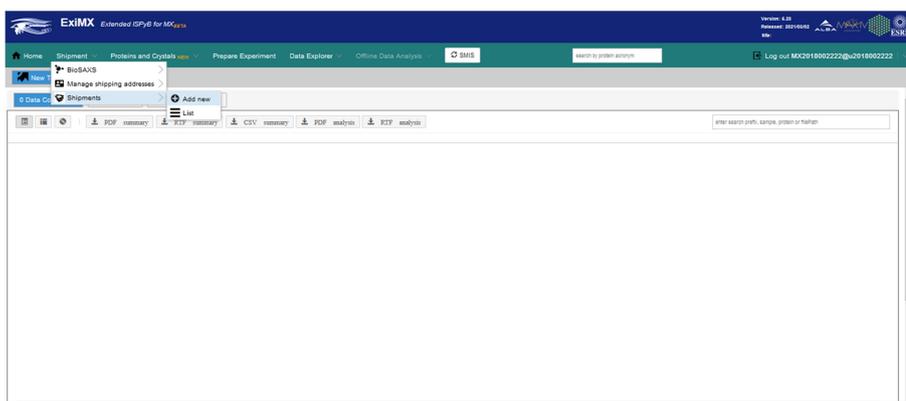
- Check the list of **lab contacts** (shipment>Manage shipping addresses>List). If none are present create one at shipment>Manage shipping addresses>Add new. The **lab contact** is the contact of your lab/Institution (Fig. 4).



- **Protein declaration:** Check if your protein has been previously declared in EXI (Proteins&Crystals>List). If needed add new ones (Proteins&Crystals>Add new protein) (Name and acronym) (Fig. 5). **This step is not mandatory for dewar shipping** and can be added afterwards when declaring the samples (see Fig.15).

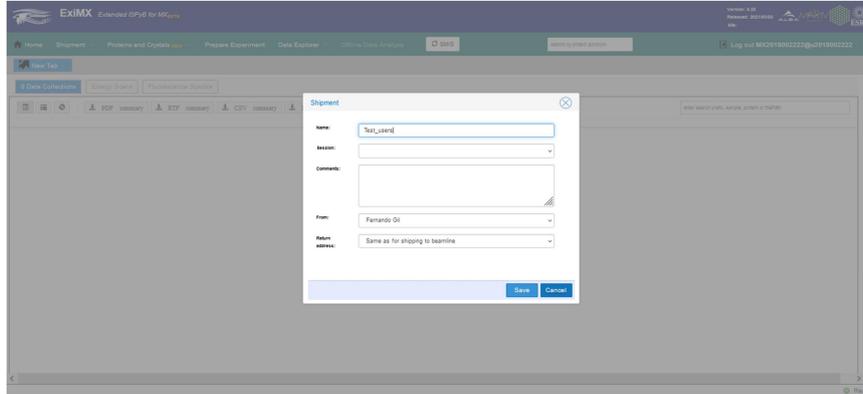


- Create a **new shipment**: To do that go to shipment in the upper menu and press Shipment>Add new (Fig. 6)

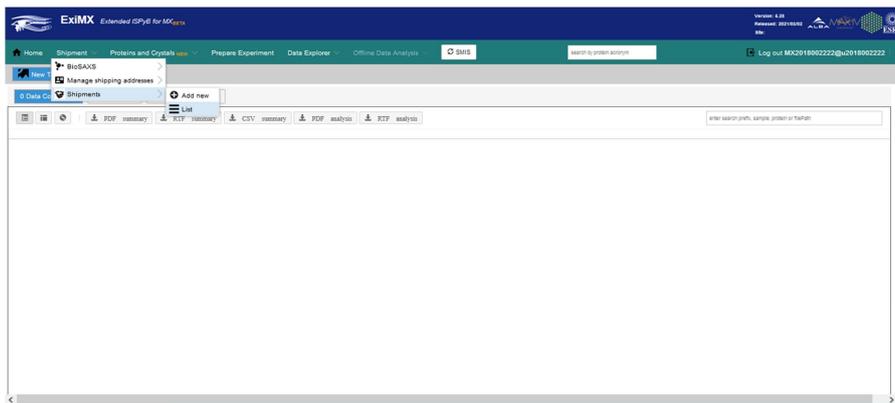




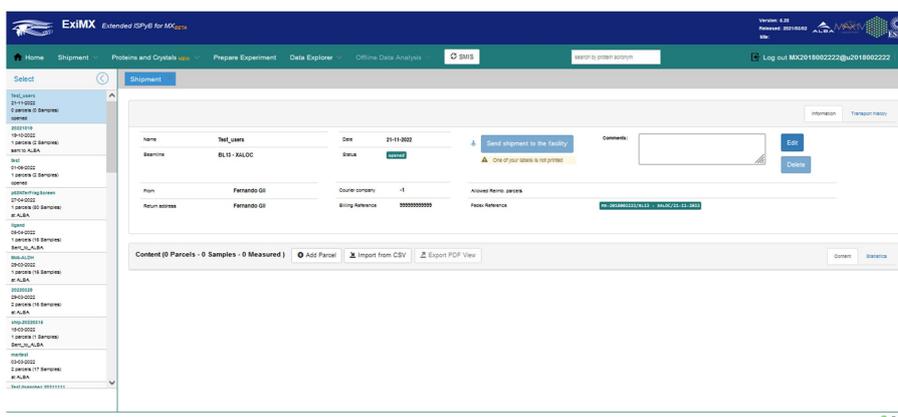
- Create the new shipment by **adding a name**, a **contact person** and **choosing the corresponding session** in the pull down menu (Fig. 7). If no session appears, contact your LC as it means your future session has still not been created.



- Go to the **list of shipments** in the Shipment menu: Shipments>list. (Fig. 8)

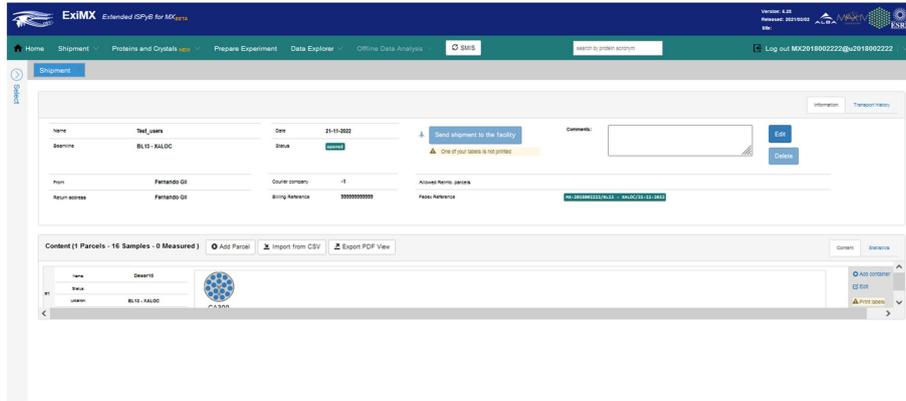


- **Select your shipment** from the list on the left. Create a dewar (“parcel” from now on) by clicking on the **Add parcel** tab. Fill it with your pucks (“containers” from now on) by choosing **Add container** in the right menu. Once created, go to the section “How to declare your samples” to fill the container. **For dewar shipping is not necessary to declare samples (but recommended) but at least you must create a parcel (minimum requirement)** (Fig. 9).

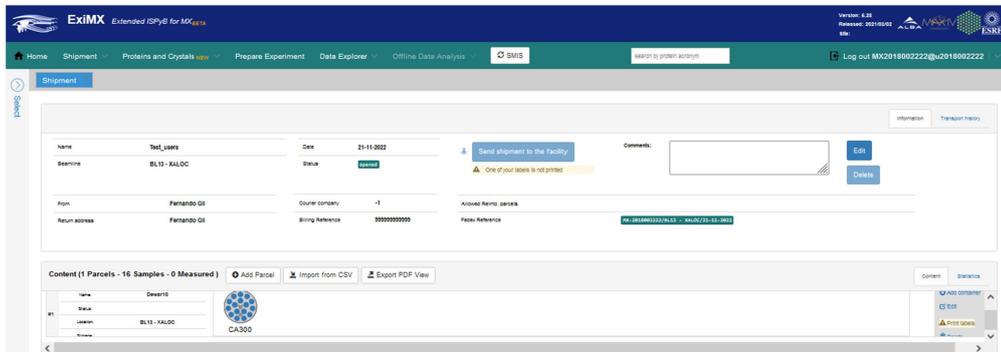




- Parcel and container with samples declared will appear as in the image below (Fig. 10).



- The next important step is to **print the labels** (right menu). Attach the two labels (send to facility and back home) to the dewar box (Fig. 11). The labels can be protected with a transparent plastic holder and attached to the dewar case. The “send to facility label” must be visible (we will replace it for the back home label when returning the dewar). Labels are essential for the courier so without them, there are high chances they do not pick up the dewar. If not possible to print the labels keep an eye to the **popup windows** in your browser.



ISPyB Dewar Tracking

LABEL INSTRUCTIONS

Please print the following three labels and use as follows:

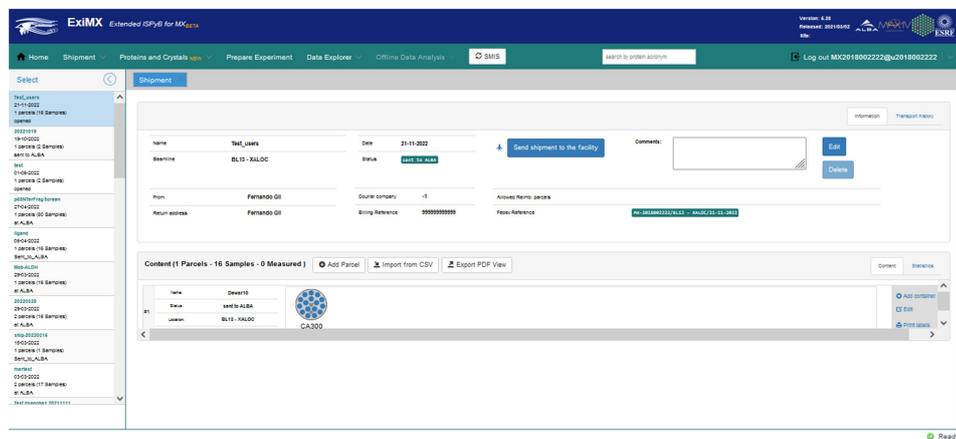
- 1) Dewar Label:** affix this label to your dewar which ensures it can be identified at all times at ALBA
- 2) Outward bound Address label:** To be attached to the outside of your transport container for shipment to ALBA
- 3) Return bound address label:** The return address for your shipment (Please include this in your shipment, e.g. put it behind the outward bound address or in the transport container)

1) DEWAR LABEL: affix this to your DEWAR

<div style="border: 1px solid black; width: 100px; height: 40px; margin-left: 10px; display: flex; align-items: center; justify-content: center;">*null*</div>	
Parcel label	Dewar10
Shipment name	Test_users
Number of parcels	1
Proposal number	MX-201800222
Laboratory name	XALOC
Local contact	



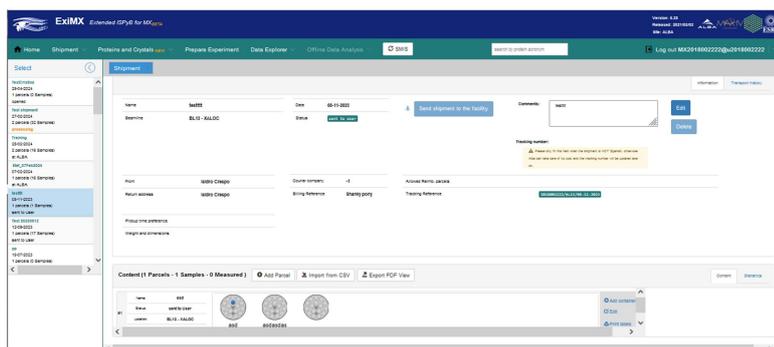
- Now a blue button is activated and you can proceed to **Send Shipment to the Facility** by pressing it. The status of the shipment will change from OPENED to SENT TO ALBA. If the blue button is not active refresh the web page or go again to Shipment>List and choose your shipment (Fig. 12).



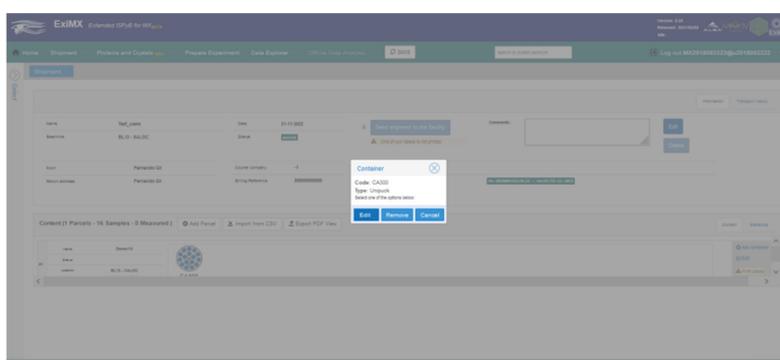
- After you press “Send Shipment to the Facility” the User Office will validate the request and will start the procedure. Shipments sent on Friday afternoon will be processed on Monday morning. The courier will pick up the dewar the following day (or even the same day if you ask the pick up very early). Keep in mind that it will take an extra day to deliver it, so the dewar should be prepared at least 2 or even 3 days (for experiments during working hours) before the experiment.

HOW TO DECLARE YOUR SAMPLES

- **Sample declaration:** For editing your samples right click over the empty container and press edit. Also if you require to inspect or modify your samples (Fig. 13).

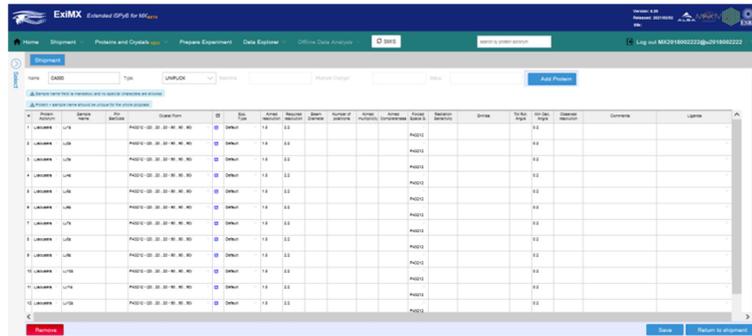


- You will see something like that (Fig. 14):

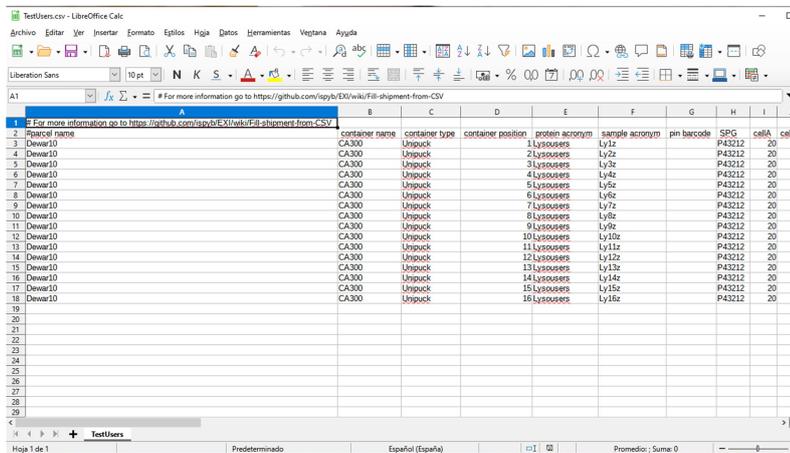




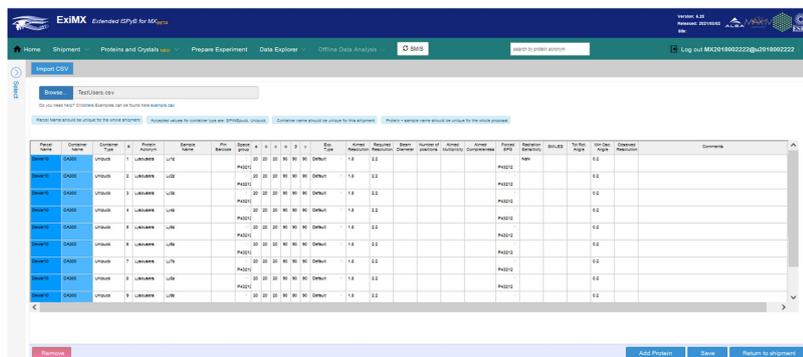
- Insert your samples by hand. If you drag with the mouse by clicking on the edge of a corner of a shell, the rest are autocompleted. Also you can add a new sample from the “Add sample” blue button. Keep in mind that **Protein+sample name must be unique for the whole proposal**, i.e. the combination Protein+sample name cannot be repeated in any of your previous beamtimes otherwise you will get an error from the application (Fig. 15).



- A second option for loading your samples is the use of a CSV template through the tab “Import from CSV” (next to the “Add parcel” tab) and filling the different fields of the file (a example.csv template is available for download). It is not required to fill everything but there are several mandatory fields. Information in columns A to F is mandatory (Fig. 16).

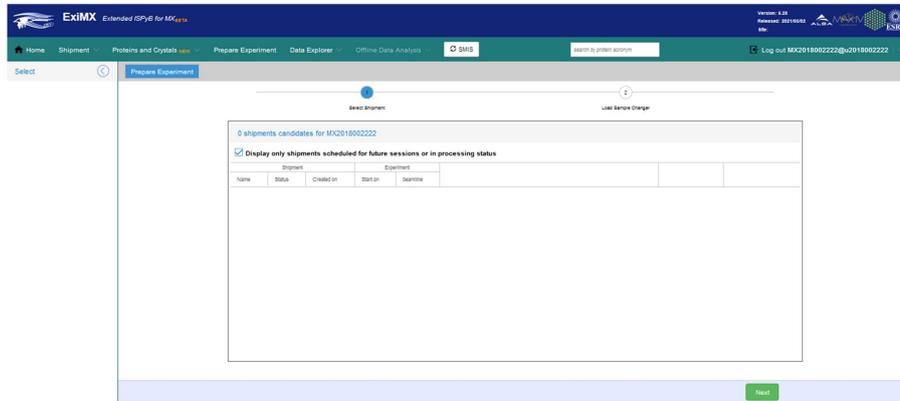


- After loading the samples, you will see all of them in EXI. Keep in mind that **Protein+sample name must be unique for the whole proposal**, i.e. the combination Protein+sample name cannot be repeated in any of your previous beamtimes, otherwise you will get an error from the application (Fig. 17).



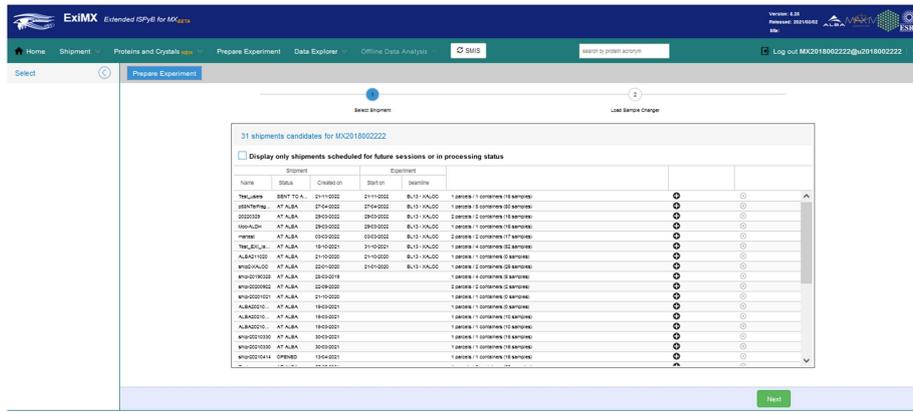
HOW TO PREPARE YOUR EXPERIMENT

- The day of your beamtime is time for **preparing your experiment**. To do that, go to

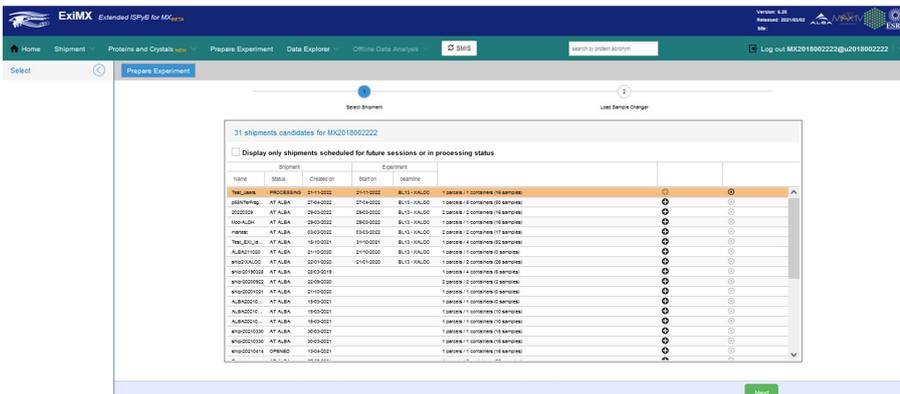


the Prepare experiment tab in the main menu (Fig. 18).

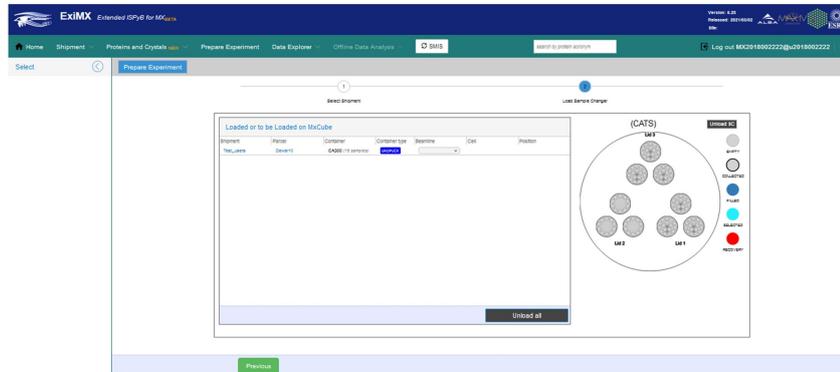
- After unclicking the “Display only shipments scheduled for future sessions or in processing status” check, you will see your shipment (Fig. 19).



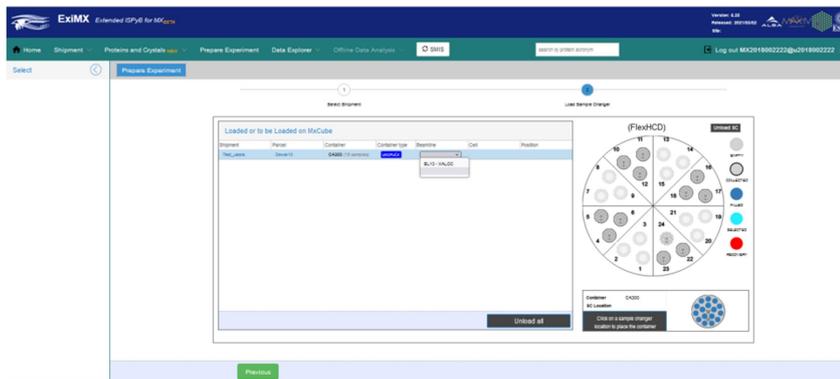
- Choose your current shipment by pressing the add icon on the right. The line will change to orange and press Next (green button below) (Fig. 20).



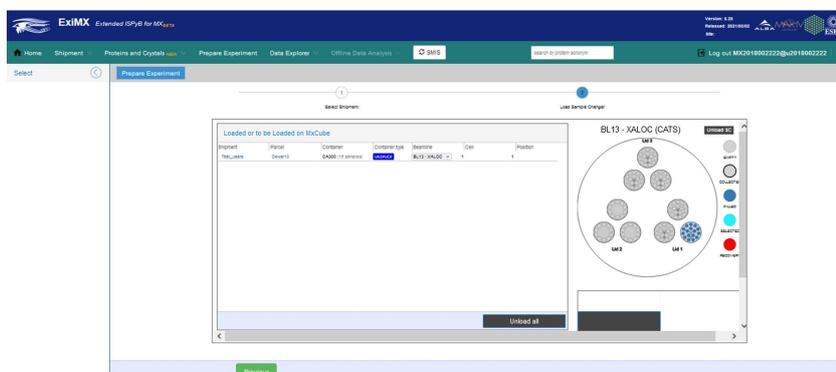
- In the second step we are going to proceed to Load the Sample Changer (Fig. 21).



- Select the appropriate beamline, in that case BL13-XALOC (Fig. 21).

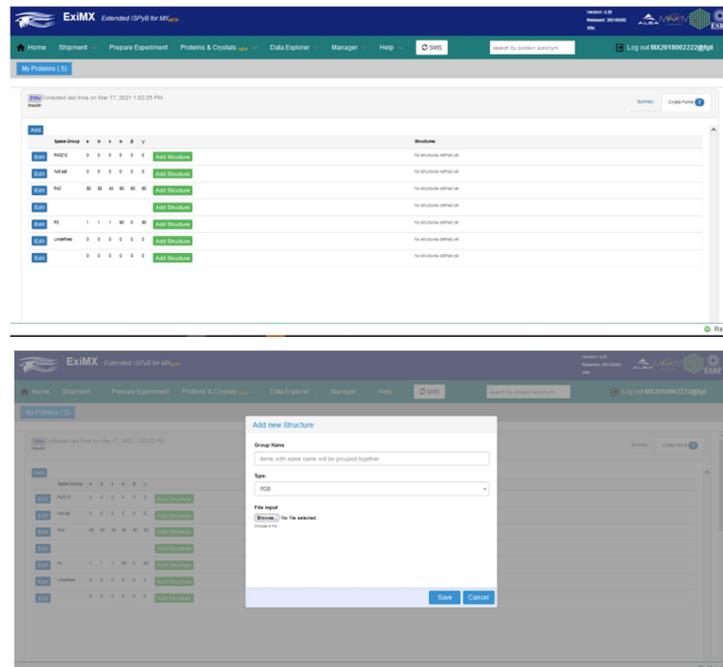


- Afterwards select the position of your pucks following the instructions of your local contact. Select the line of your container and then press the corresponding position of the sample changer. This information will be added to your container (cell, position) (Fig. 22).





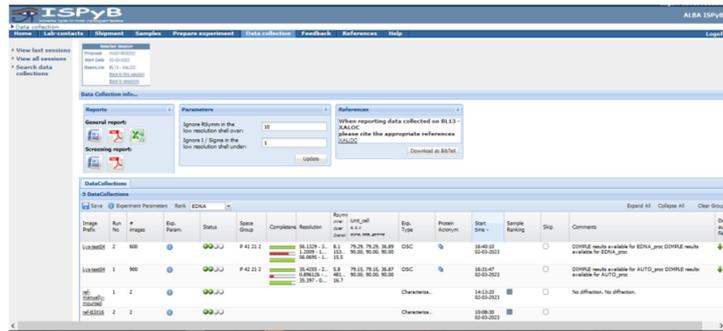
- At any time before the data collection you can add a PDB code of your protein for MR (Dimple). Go to the tab Proteins&Crystals>List. Go to a protein previously declared and click the “Crystal forms” tab. Press the “Structure” button corresponding to your crystal form and upload the PDB code (Fig. 23).



- Download your Dimple results from:
 - Enter to your ISPyB session in the Home page
 - Go to the data collection of interest (OSC). If Dimple processing worked nicely you will find the comment: “DIMPLE results available for EDNA_proc
DIMPLE results available for AUTO_proc”
 - Click the “Last collected results” tab.
 - Click the autoPROC or EDNAproc processing. You will find the Dimple outputs at the “Attachments” section.
- Done!

TROUBLESHOOTING

- How can I download a summary of my experiment in .csv format?
 - For the moment this option is not available in EXI, however temporarily you can download the .csv summary from the old version of ISPyB (www.ispyb.cells.es/ispyb): Login>Press GO at MX proposal>Press Data Collection tab>View collections>Reports (first panel above)



The screenshot shows the ISPyB web interface. The top navigation bar includes 'Home', 'Lab contacts', 'Shipment', 'Samples', 'Prepare experiment', 'Data collection', 'Feedback', 'References', and 'Help'. The left sidebar has 'View last sessions', 'View all sessions', 'Export data', and 'Collections'. The main content area is divided into 'Data Collection Info' and 'Data Collections'.

Data Collection Info:

- Reports:** Includes 'Manual report', 'Screening report', and 'Parameters'.
- Parameters:** Fields for 'Ignore XRDs in the log receptor that are:' (set to 10) and 'Ignore / Ignore in the log receptor that are:' (set to 1). A 'Update' button is present.
- References:** Text: 'When reporting data collected on BL13: AALOC - please use the appropriate references: COLCOC'. A 'Download as CSV' button is available.

Data Collections Table:

Stage	Run	Exp. Param.	Status	Speed	Completion	Resolution	Apert.	Exp. Type	Protein	Sample	Skip	Comments
1	1	100	Completed	10000	100%	2.0	10.0	OSC				COMPRE results available for ECDNA, please COMPRE results available for ECDNA, please
1	2	100	Completed	10000	100%	2.0	10.0	OSC				COMPRE results available for AUTO, please COMPRE results available for AUTO, please
1	1	100	Completed	10000	100%	2.0	10.0	Characterization				No diffraction, no diffraction.