

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



ExiMX Extended SPyE for MX ===	
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Login	$\otimes$
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	ummaread
	Please use your DUO login Login
	Resty.

- Login to EXI using the credentials of your proposal
- In order to load your samples in EXI, first enter in the session corresponding to your beamtime (in the example shown, 21/11/2022)

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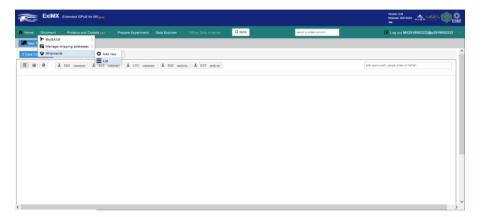
- Create a new shipment: To do that go to shipment in the upper menu and press Shipment>Add new

EXIMX Extended (SPyE) for Million	
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- Create the new shipment by adding a name, a contact person and choosing the corresponding session in the pull down menu.

ExIMX Extended GPy6 for MX <sub>1278</sub>				MANNA AND AND AND AND AND AND AND AND AND
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- Go to the list of shipments in the Shipment menu: Shipments>list.



- Select your shipment from the list on the left. Now it is time to load your parcel (dewar) and samples information in EXI.



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- The easier option to load your samples would be the use of the CSV template provided (here) filling the different fields. It is not required to fill everything but there are several mandatory fields. Information in columns A to F is mandatory.

TestUsers.csv - LibreOffice Calc								-	
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- Use the "Import from CSV" option to load your CSV file.

ExiMX Exte	ended ISPyB for MX <sub>SCIN</sub>			
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- 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. Protein +

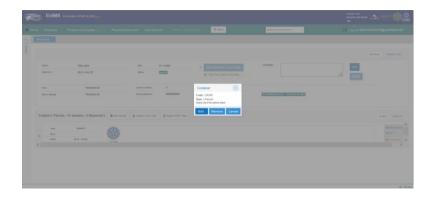
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sample name cannot be repeated in any of your previous beamtimes otherwise you will get an error from the application.

- Now you can Return to Shipment where you will find your dewar and samples declared.

ExiMX (	Ixtended ISPy8 for MK <sub>861A</sub>						Versier 631 Reference 20210500 ALBANIMENT
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- Later on you can inspect or modify by editing your samples through right click on the basket shown.





- Once you are happy with your samples it is time to send the shipment to the facility but first you have to print the labels (menu on the right of the samples) and attach it to the dewars.

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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
forshipment to ALBA
3) Return bound address label: The return address for your shipment (Please include this in
yourshipment, e.g. put it behind the outward bound address or in the transport container)

	1) DEWAR	LABEL: affix this to your DEWAR
ALBA	*null*	
	Parcel label	Dewar10
	Shipment name	Test_users
	Number of parcels	1
	Proposal number	MX-2018002222
	Laboratory name	XALOC
	Local contact	



- Now you can proceed to Send Shipment to the Facility by pressing the blue button. 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.

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es di Sarones A	Content (1 Parcels	- 16 Samples - 0 Measured)				© Add container ES Exel

- When the day of your beamtime has arrived it is time for preparing your experiment. To do that, go to the Prepare experiment tab in the main menu.

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- After unclicking the "Display only shipments scheduled for future sessions or in processing status" check, you will see your shipment.

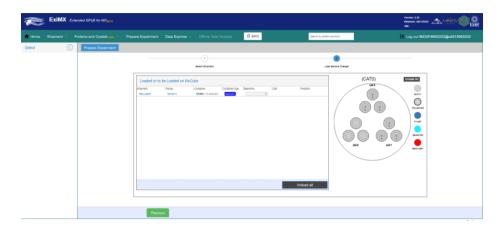
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		AL8A20210	AT ALBA	19-03-0021			1 percets / 1 containers (10 samples)		0	•		
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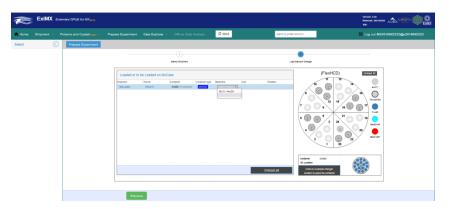
- Choose your shipment by pressing the add icon on the right. The line will change to orange and press Next (green button below)

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- In the second step we are going to proceed to Load the Sample Changer.

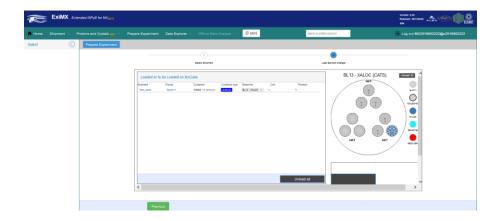


- Select the appropriate beamline, in that case BL13-XALOC





- Afterwards choose the position of your pucks following the instructions of your local contact.



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

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- 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 versión of ISPyB (www.ispyb.cells.es/ispyb): Login>Press GO at MX proposal>Press Data Collection tab>View collections>Reports (first panel above)

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