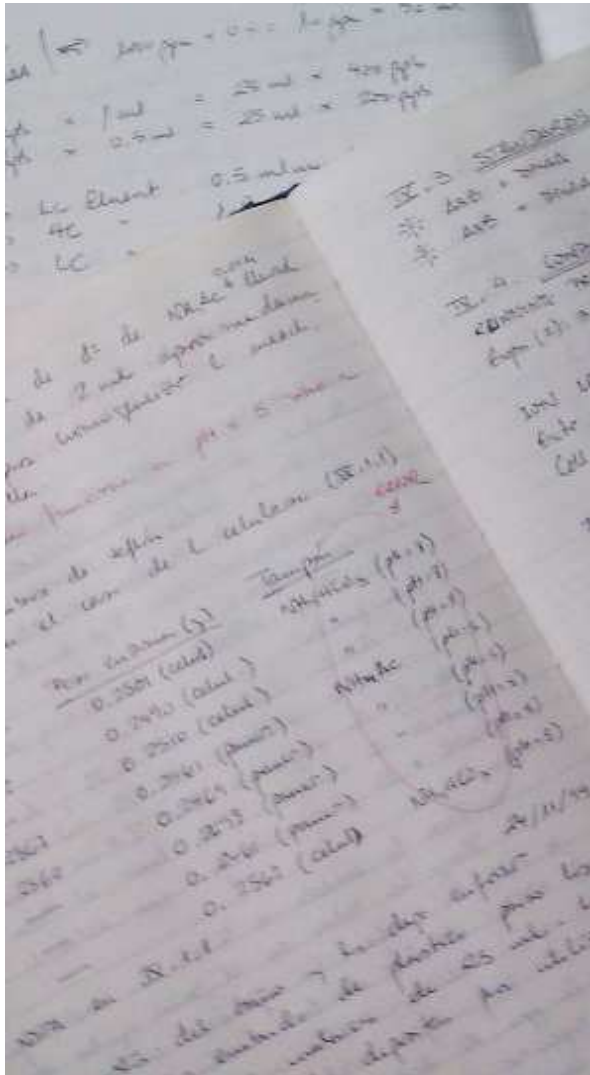




# EXI : a new interface for ISPyB

S. Monaco



## The structural biologist's experiment companion:

- **Sample tracking** to or from the synchrotron
- **Electronic logbook** for MX and BIOSAXS
  - experiments assisting users (sample list, results view, complex experiments overview)
  - source of information for automatic experiments (MASSIF-1)
  - the memory of a project

## ISPYB : OFFICIAL PAN-EU COLLABORATION

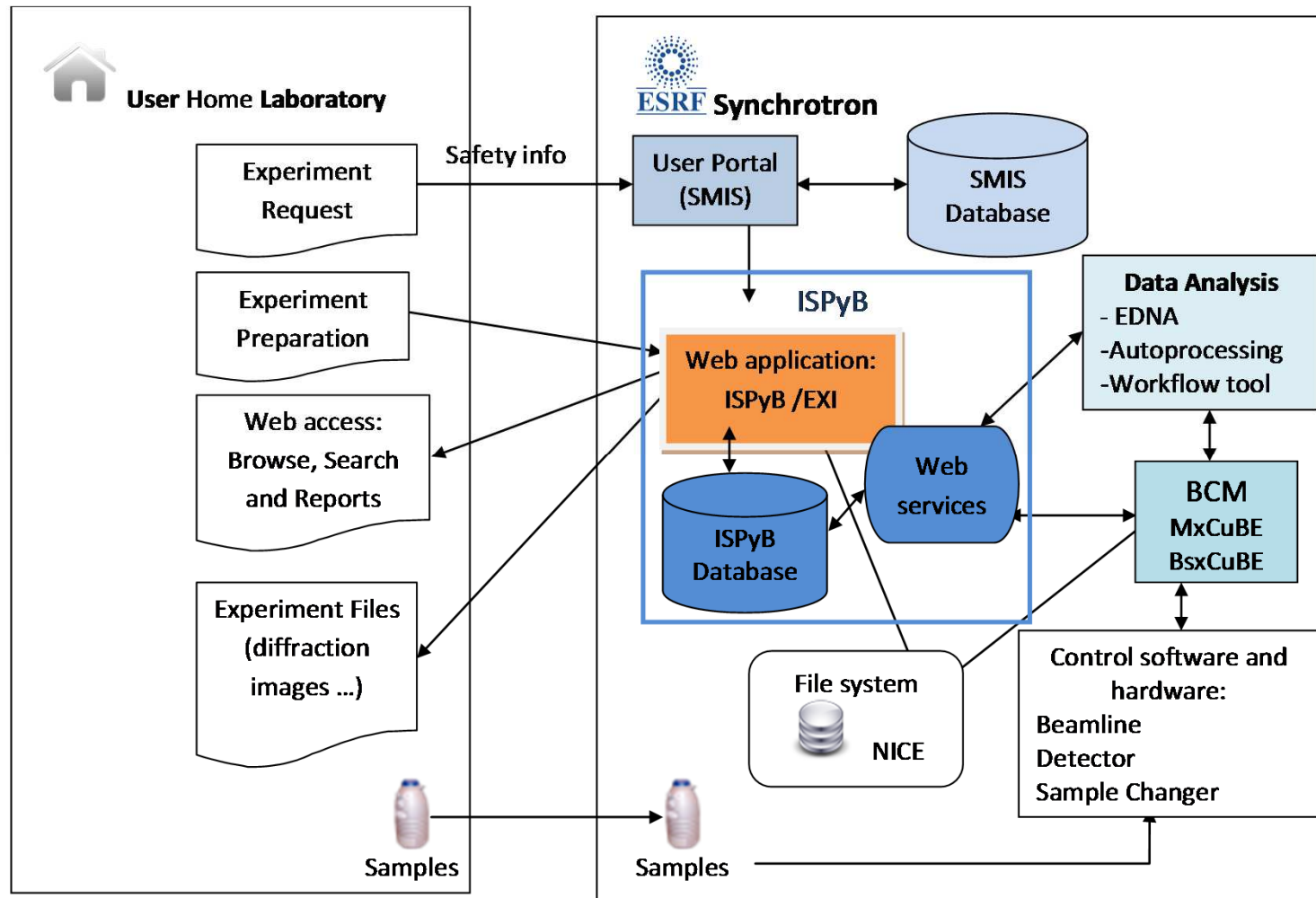


Collaboration agreement contract signed in **January 2017** by **8 sites** :

- Real wish to develop together (share manpower resources)
- To provide the same results/tools to our user communities



# EXI : EXTENDED ISPYB



EXI : same Java technology as ISPyB GUI



- **Faster display** of summary page especially with complex workflows (WF)
- No going back and force to other pages to visualize more details
- **Intuitive** accesses to avoid manual reading
- **Simplification** of the processes (vs. an interface evolving over 10 years with multiple add-ons)

# EXI MX : ENRICHMENT OF THE SESSION SUMMARY PAGE

ExiMX Extended ISPyB for MX<sub>BETA</sub> Version: 0.9.8  
Released: 2016/12/22

Home Shipment Proteins and Crystals Prepare Experiment Data Explorer Offline Data Analysis Help  Log out MX1862@smnaco

---

New Tab

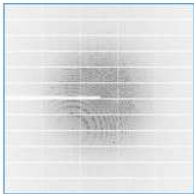

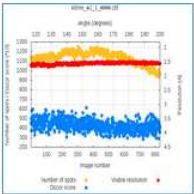
Very weak diffraction.

---

**Run #1 OSC** Dec 15, 2016 8:51:38 AM  
/data/visitor/mx1862/029/20161215/RAW\_DATA

Summary Beamline Parameters Data Collections **1** Sample Results **15** Workflow

Workflow	Type	OSC	P 42 21 2	Completeness	92%	Res.	3.7	Rmerge	3.7
Protein	Res. (corner)	1.3 Å (1.07 Å)	Inner	98%	1.3	82.6			
Sample	Wavelength	0.977 Å	Outer	97%	1.3	9.0			
Prefix	Phi range	0.1 °	Overall						
Images	Phi start (total)	200° (83°)	cell A	cell B	cell C				
Transmission	Exposure Time	0.037 s	67.2964	67.2964	100.883				
Flux start	Flux end	2.02e+11 ph/sec	Alpha	Beta	Gamma				
			90	90	90				



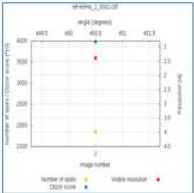





---

**Run #1 Characterisation** Dec 15, 2016 8:48:48 AM  
/data/visitor/mx1862/029/20161215/RAW\_DATA

Summary Beamline Parameters Data Collections **1** Sample Results Workflow **1**

Workflow	Type	Characterisation	Indexed	Mosaiicity	0.45	
Protein	Res. (corner)	1.3 Å (1.07 Å)	Strategy	Space Group	P4	
Sample	Wavelength	0.977 Å	Rank Res.	1.33 Å	Exp. Time	0.037 s
Prefix	Phi range	1 °	Images	830	Total rotation	0.1 °
Images	Phi start (total)	540° (180°)	Transmission	7.3324		
Transmission	Exposure Time	0.037 s	cell A	cell B	cell C	
Flux start	Flux end	2.5e+12 ph/sec	67.25	67.25	100.66	
			Alpha	Beta	Gamma	
			90	90	90	









---

**Run #2 Characterisation** Dec 15, 2016 8:45:46 AM  
/data/visitor/mx1862/029/20161215/RAW\_DATA

Summary Beamline Parameters Data Collections **1** Sample Results Workflow

Workflow	Type	Characterization			
----------	------	------------------	--	--	--

# EXI MX: SESSION SUMMARY

Run #1 OSC Jul 20, 2016 4:23:03 PM  
/data/visitor/mx415/id30b/20160720/RAW\_DATA/therm/therm-t07

Summary Beamline Parameters Data Collections 9 Sample Results 18 Workflow 6

Workflow	MXPressE	Type	OSC	P 4 2 2	Completeness	Res.	Rmerge		
Protein	therm	Res. (corner)	1.08 Å (0.94 Å)	Inner	98%	3.0	1.3		
				Outer	99%	1.1	83.0		

Run #1 OSC Jul 20, 2016 4:23:03 PM  
/data/visitor/mx415/id30b/20160720/RAW\_DATA/therm/therm-t07

Summary Beamline Parameters Data Collections 9 Sample Results 18 Workflow 6

Run	Prefix	#images	Exposure Time	Res. (corner)	Wavelength	Transmission	Directory	Time	Run status	Phasing
#1										
#1										
#1										

Run #1 OSC Jul 20, 2016 4:23:03 PM  
/data/visitor/mx415/id30b/20160720/RAW\_DATA/therm/therm-t07

Summary Beamline Parameters Data Collections 9 Sample Results 18 Workflow 6

InnerShell Overall OuterShell

Home Shipment Proteins and Crystals Prepare Experiment Data Explorer Offline Data Analysis Help

search by protein acronym Log out MX415@smonaco

Run #1 OSC Jul 20, 2016 4:23:03 PM  
/data/visitor/mx415/id30b/20160720/RAW\_DATA/therm/therm-t07

Summary Beamline Parameters Data Collections 9 Sample Results 18 Workflow 6

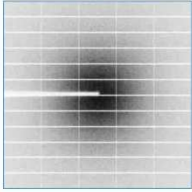
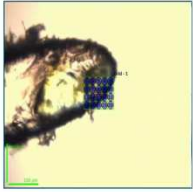
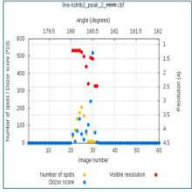
Snapshots	Automesh	Mesh	Line	Characterisation	Characterisation
Success	Success	Success	Success	Success	Success

3.6 2.0 3.6 2.0 merged\_anom\_XSCALE.LP

# EXI MX: STRUCTURE SOLUTION OF SAD PHASING

**New Tab**

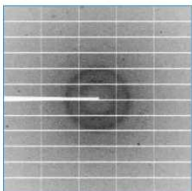
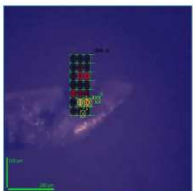
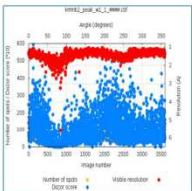
Workflow	<b>XrayCentering</b>	Type	<b>Helical</b>
Protein		Res. (corner)	<b>1.49 Å (1.16 Å)</b>
Sample		Wavelength	<b>0.863 Å</b>
Prefix	<b>line-kdmb2_peak</b>	Phi range	<b>0.0508333 °</b>
Images	<b>80</b>	Phi start (total)	<b>182.056° (3.06°)</b>
Transmission	<b>36.9312</b>	Exposure Time	<b>0.1 s</b>
Flux start	<b>1.99e+11 ph/sec</b>	Flux end	<b>2.03e+11 ph/sec</b>

**Run #1\_05C** Dec 15, 2016 12:26:46 PM  
/data/visitor/mx1862/d29/20161215/RAW\_DATA/KR/KmMB2/PEAK

[Summary](#) [Beamline Parameters](#) [Data Collections](#) **1** [Sample](#) [Results](#) **12** [Workflow](#) [Phasing](#) **29**

Workflow		Type	<b>OSC</b>	<b>P 1 21 1</b>	<b>Completeness</b>	<b>Res.</b>	<b>Rmerge</b>
Protein		Res. (corner)	<b>1.21 Å (0.98 Å)</b>	Inner	<b>100%</b>	6.3	3.0
Sample		Wavelength	<b>0.863 Å</b>	Outer	<b>97%</b>	1.4	83.9
Prefix	<b>kmmb2_peak_w1</b>	Phi range	<b>0.1 °</b>	Overall	<b>98%</b>	1.4	9.2
Images	<b>3600</b>	Phi start (total)	<b>360° (360°)</b>	<b>cell A</b>	<b>cell B</b>	<b>cell C</b>	
Transmission	<b>4.15006</b>	Exposure Time	<b>0.037 s</b>	34.2	30.7	63.7	
Flux start	<b>2.3e+10 ph/sec</b>	Flux end	<b>3.07e+10 ph/sec</b>	<b>Alpha</b>	<b>Beta</b>	<b>Gamma</b>	
				90	105.3	90	

Automatic SAD appears to have worked with the space group P1211

**Run #1 Characterization** Dec 15, 2016 12:24:30 PM  
/data/visitor/mx1862/d29/20161215/RAW\_DATA/KR/KmMB2/PEAK

[Summary](#) [Beamline Parameters](#) [Data Collections](#) **1** [Sample](#) [Results](#) [Workflow](#) **1**



Ready



# EXI MX : SAMPLE DESCRIPTION

Description of more generic shipment to fulfill all Beamline needs (plates, liquid, spine, unipucks..) – *under validation*

ExiMX Extended ISPyB for MX<sub>BETA</sub> Version: 0.9.8 Released: 2016/12/22 ESRF

Home Shipment Proteins and Crystals Prepare Experiment Data Explorer Offline Data Analysis Help search by protein acronym Log out mx415@mx415

Shipment

Name: unL\_1 Type: UNIPUCK Beamline: #Sample Changer: Status:

#	Protein Acronym	Sample Name	Crystal Form	Exp. Type	Pin BarCode	Pre-observed resolution	Needed resolution	Pref. Diameter	Number Of positions	Radiation Sensitivity	Required multiplicity	Required Completeness	Space Group	Smiles	Comments	Edit Crystal Form
1	N15SH		P65 - (0 : 0 : 0   90 : 90 : 120)			0	0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
2	N15SH		P65 - (0 : 0 : 0   90 : 90 : 120)			0	0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
3	N15SH		P65 - (0 : 0 : 0   90 : 90 : 120)			0	0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
4	N15SH		P65 - (0 : 0 : 0   90 : 90 : 120)			0	0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
5	N15SHD		P21			0	0	0	0	0	0	0	P21			<a href="#">Edit Crystal Form</a>
6	N15SH		P65 - (0 : 0 : 0   90 : 90 : 120)			0	0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
7	N15SH		P65 - (0 : 0 : 0   90 : 90 : 120)			0	0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
8																
9																
10																
11																
12																
13																
14																
15																
16																

Remove Save Return to shipment

Ready Ready

# EXI MX: SYNCHRONISATION WITH MXCUBE PREPARATION

ExiMX Extended ISPyB for MX

Home Shipment Proteins and Crystals Prepare Experiment Data Explorer Offline Data Analysis Help

search by protein acronym Log out mx415@mx415

Prepare Experiment

1 Select Shipment 2 Load Sample Changer

Shipment	Container	Barcode	Container type	Beamline	Sample Changer Loc...
slp1	CA45 (3 samples)	ESRF020070	UNIFLEX	ID30B	
slp1	ca45 (7 samples)	ESRF020071	UNIFLEX	ID30B	
Wf-astrocytes	pu4C (10 samples)	ESRF020034	SPENERUCE	ID30-2	1
Wf-astrocytes	pu4C (10 samples)	ESRF020034	SPENERUCE	ID30A-3	
Wf-astrocytes	pu4C (10 samples)	ESRF020034	SPENERUCE	ID30-2	
Wf-astrocytes	pu4C (10 samples)	ESRF020034	SPENERUCE	ID30-2	
Wf-astrocytes	pu4C (10 samples)	ESRF020034	SPENERUCE	ID30-2	

Unloaded all

ID30B (FlexHCD)

Container: ca45  
SC Location:

Click on a sample changer location to choose the devar

- Simplification
- Management of multiple sample changers of the ESRF SB beamlines

# EXI BIOSAXS SINCE JAN 2016

The screenshot displays the ExiSAXS software interface, which is an extended ISPyB for SAXS. The interface is divided into several sections:

- Header:** Shows the ExiSAXS logo, the text "Extended ISPyB for SAXS BETA", and the version information "Version: alpha Released: 2017/01/27".
- Navigation:** Includes a menu with "Home", "Shipment", "Prepare Experiment", "Data Explorer", and "Help". A search bar for "search macromolecule" and a "Log out MX1848@smon" button are also present.
- Browse by:** A sidebar on the left lists various experiments and samples, including "FAPGNAPAL", "FAPGWYPAL", "MAANAAM", and "CALIBRATION".
- Data Collection Table:** A central table displays data for various runs. The columns include Run, Sample, Frames (Average/Total), Rg, Points, I0, Rg Total, D<sub>max</sub>, Volume, MM Vol. est., Scattering, Kratky, Density, Guinier, and Advanc. The table shows data for runs HPLC\_B, HPLC\_M, and HPLC\_C.
- Plots:** The interface includes several plots: a "Deep Well" plot showing a grid of circles, and a "Size-exclusion chromatography" plot showing a single peak at a volume of approximately 1.7. The chromatography plot includes a legend with items like I0, sum\_I, Rg, Mass, Vc, Qr, and quality.
- Right Panel:** Contains a "Data Red" section with checkboxes for "Abel", "Fit", "Superp", and "Rigid B".

## PLAN FOR EXI FOR THE STRUCTURAL BIOLOGY COMMUNITY



### **MX:**

- Beta testers for feedback once all major tools in place
- Open to all MX community
- MR results display
- Presence of ligand probability (INEXT)
- Off line data processing : DIMPLE, “mesh & collect” HCA

### **BIOSAXS:**

- Finish polishing existing pages
- New developments for membrane proteins (INEXT, SOLEIL and EMBL HH)

### **CryoEM:**

Database work done by DLS – EXI webpages to come

**EXI in general:** retrieve results from multiple techniques, from multiple sites

# HOW TO ACCESS IT?



**ExiMX** *Extended ISPyB for MX<sub>BETA</sub>*

<https://exi.esrf.fr/>

Login



User:

Password:

**Demo on MASSIF-3  
this afternoon**

## EXI : A SPECIAL THANKS TO

- Alejandro de Maria
- Sergio Gonzales
- Solange Delagenière
- Olof Svensson
- All ESRF Automation Task Force members  
D. Van Stetten, M. Nanao, A. Mc Carthy (EMBL), M. Bowler (EMBL), M. Brennich (EMBL), P. Pernot
- Gordon Leonard
- Marcin Wojdyr (DLS) for Uglymol