



# Towards standard APIs for the exchange of meta data between homelab LIMS software and ISPyB

ISPyB-developers meeting Berlin, October 2019

Rik Wierenga FBMM, BCO University of Oulu Oulu Finland



Towards standard APIs for the exchange of meta data between homelab LIMS software and ISPyB

Oulu (Rik Wierenga)

Weizmann (Joel Sussman)

Diamond (Alun Ashton)



IceBear:

Integrated Crystal-data-tracking Enhancing Biochemistry Education And Research

Developed by Ed Daniel (University of Oulu)

Addressing the needs of the researchers of a homelab, using a diverse range of crystallization setups and crystal treatment protocols.



Icebear version 1.1.0 Distributed under the MIT Licence



- 1 Crystallization and diffraction meta data in one data base
- 2 Meta data of crystals-on-pins
- 3 Link from the ISPyB shipment is stored in the homelab data base

We need to capture the workflow for cryofreezing selected crystals of selected drops --connecting crystals to pins(barcoded/puckpositioned) --cleaning/recycling dewar contents when the dewar comes back

We need to upload the meta data to ISPyB such that data collection can be done

We want to retrieve the link where ISPyB will store the diffraction information

We use barcoded pins, but the protocol will also work with non-barcoded pins

We have written a rapid-access proposal to Diamond to test these protocols on the live-server at Diamond and we have tested this now in two sessions.



Icebear: https://icebear.oulu.fi/shipment/13899966 Diamond Light Source: https://ispyb.diamond.ac.uk/shipments/sid/31948





Shipment: DLS 12 Oct Dewar 1

To: Diamond Light Source

Shipped: 2019-10-04

## Dewar DLS-MX-0643, puck CPS-4618

1	HA00AS6602	rpMFE1_95brC02d2c1	
	Icebear		Diamond Light Source
	HA00AS6876	rpMFE1_95brC02d2c2	
	Icebear		Diamond Light Source
2			
	HA00AR7699	rpMFE1_95brC02d1c1	

Advantages, from the homelab perspective:

In Oulu there are about 30 researchers, newcomers very regularly starting

All researchers have direct access to the crystallization facility

Education: the information now provided by the system makes it much easier for supervisors to monitor/discuss the crystallization results and diffraction information as well as using the power of the processing and structure determination pipelines running at the ESRF and DLS

Research: All important data of the structure determination pipeline can now be recorded in one data base and are then available when writing publications

One person is needed to coordinate the shipment.

Inexperienced users are easily trained. Returning dewars are routinely cleaned.

Advantages, from the synchrotron perspective:

Proposal numbers, session numbers, beamline, data collection dates can be recorded. Any PDB-ident can be connected to where and when the data set was collected. Better use of the processing and structure determination pipelines.

The optimal use concerns a lab that has Formulatrix imagers driven by Rockmaker.

The software can be installed remotely using an installer.

Upgrades can be dowloaded and implemented easily.

-we would like to upload more information: to optimally benefit from the data-processing-pipelines and the structure-determination-pipelines at the ESRF and DLS (sequence, structure/PDB-chain, ligand).

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overall	661228		190033	2.17 - 65.30	0.070	8.6 1	0	99.1	3.5	93.5	1.8	-0.4

Downstream Processing

Fast EP: ? Dimple: ? MrBUMP: ? Big EP/XDS: ? Big EP/DIALS: ?

Practical aspects of how the work flow is captured

Search for plates, but also for dewars, crystal-identifiers, pin-barcodes



## Find by barcode...

Drotei

LmTIM Construct: LmTIM-E65Q \$?∎

Well solution 1.75M (NH4)2HPO4 Screen: Factorial1

Protein solution Protein concentration: 50mg/mL Protein buffer: Example buffer

Drop volumes Protein solution: 100nL Well solution: 100nL

Plate Type: Corning flat 1 Drop Barcode: 9098

Incubation Imager: +20 RI54 Temperature: 20°C



Trial drop viewer: Plate <u>9098</u> drop A01.1



## Find by barcode...

# \$? ∎

#### Protein

LmTIM Construct: LmTIM-E65Q

#### Well solution

1.75M (NH4)2HPO4 Screen: Factorial1

#### **Protein solution**

Protein concentration: 50mg/mL Protein buffer: Example buffer

#### **Drop volumes**

Protein solution: 100nL Well solution: 100nL

#### Plate

Type: Corning flat 1 Drop Barcode: 9098

#### Incubation

Imager: +20 RI54 Temperature: 20°C





(selecting a crystal: crystal identifier/sample name: LMTIM\_9098A01d1c1)

"fishing" module: we need to connect a crystal to a pin-barcode / position-in-puck

"shipment" module: to sent the meta data to ISPyB and clean the returning dewar

"crystal-page" module: to make accessible the ISPyB-link, DOI of the raw data, PDB entry



Freezing crystals: barcode reader is used to identify pins, pucks and dewars touch screen (or mouse) is used to record that a crystal has been attached to a pin



Using IceBear when freezing crystals:

a crystal gets associated with a pin/pinbarcode or pin/puck position

## Shipment: Shipment for test

Shipment OUL-XX-9999		
Shipment details		Your shipment at Diamond Synchweb Live
Name	Shipment for test The name of the shipment	Open shipment in new tab
Destination	Diamond Synchweb Live Where the shipment is sent	
Shipper	System Administrator The local person responsible for the shipment	

Today

Date shipped

ISPyB link is recorded in the data base. Other info (proposal-ID, session-ID, beamline-ID) can also be recorded.

Find by barcode...

		🤮 diamond		
Proposals	No Proposal ≽		Feedback	Help
Please note that all dewars m	nust now be registered before creating a ship	oment. Please see the updated help pages for details of the new process.		×
Please note that all dewars m	nust now be registered before creating a ship	oment. Please see the updated help pages for details of the new process.		×
Please note that all dewars m	nust now be registered before creating a ship	ment. Please see the updated help pages for details of the new process.		×
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Please note that all dewars m LOGIN Username (FedID) Password	uust now be registered before creating a ship	oment. Please see the updated help pages for details of the new process.		20

#### SynchWeb? What is This?



e 🚺 Logout				👥 diamond			
ts » Shipment for test » Co	ontainers » OUL-9999						
	Proposals	mx4025 ≽	Projects	Unit Cell Search	Feedback	Help	
	Please note that all dewars must no	w be registered before creating a ship	oment. Please see the updated help page	es for details of the new process.		×	
	Container: OUL-99	999					
	This page shows the contents of the	e selected container. Samples can be	added and edited by clicking the pencil ic	on, and removed by clicking the x			_
							•
	Shipment		Shipment for test				
	Dewar		OUL-XX-9999		7	6 16	
	Container Type		Puck				
	Registered Container		Oliok to adit		8	1 15	
	Registered Container				2	5	
	Barcode		OUL-9999		9	14	
	Automated Collection		+ Queue this container for Auto Col	lect	3		
	Comments		Click to edit		10	13	
	Location History		Date Status Location Beamline		11	12	
	Location motory		No history found				
			10 🔻 Page « ( 1 )	· »			

Location	Protein Acronym	Name	Spacegroup	Barcode	Comment	Anomalous	Abundance	Components	Required Res	Unit Cell	Sta	tus
1	LMTIM	LMTIM_9098B02d1c1	C222	OU99XX9999	Shoot this one first					A B C α 100 100 100 90	β γ 90 90	ø Q
2												Ø
3												ø
4												ø
5												ø
6												A



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	Icebear		Diamond Light Source
2			
	HA00AR7699	rpMFE1_95brC02d1c1	

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Crystal: LMTIM_9098A01d1c1		Find by ba	arcode			
Crystal Final Crystal Crystal Show in drop viewer Plate 9098	Protein Data collections Files Notes   Shipment: Shipment for test to Diamond Synchweb Live, shipped 12 May, returned 13 May View shipment at Diamond Synchweb Live   View crystal at Diamond Synchweb Live View crystal at Diamond Synchweb Live View crystal at Diamond Synchweb Live					

The crystal page



Trial drop viewer: Plate <u>9098</u> drop A01.1



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#### **Drop volumes**

Protein solution: 100nL Well solution: 100nL

#### Plate

Type: Corning flat 1 Drop Barcode: 9098

#### Incubation

Imager: +20 RI54 Temperature: 20°C



IceBear WWW-based viewer of the crystallization results

	🧏 Shi	pment: TestRetu	Find b	y barcode								
Shipm	hipment DEWAR1 Files Shipment return											
Θ	Dewar DEWAR1: 1 puck is still in this dewar.											
E	Puck P	PUCK1: Crystals to keep,		Remove puck from dewar								
	Pos	Pin	Crystal	Protein	Action on return							
	1	PIN1	w_4000B01d1c1	LMTIM	Wash pin	Remove and Keep crystal Wash pin						
	2	PIN2	w_4000B01d1c2	LMTIM	Keep crystal	Remove and Keep crystal Wash pin						
	3	PIN3	w_4000B01d1c3	LMTIM	Wash pin	Remove and Keep crystal Wash pin						
	4	PIN4	w_4000B01d1c4	LMTIM	Keep crystal	Remove and Keep crystal Wash pin						
	5	(no barcode)	w_4000B01d1c5	LMTIM	Wash pin	Non-barcoded pin. Remove and wash						
	6	(no barcode)	w_4000B01d1c6	LMTIM	Wash pin	Non-barcoded pin. Remove and wash						
	7	(no barcode)	w_4000B01d1c7	LMTIM	Wash pin	Non-barcoded pin. Remove and wash						
	8	(no barcode)	w_4000B01d1c8	LMTIM	Wash pin	Pin removed and washed.						
	9											
	10											
	11											
	12											
	13											
	14											
	15											
	16											

# Cleaning/recycling of the dewar and its contents when the dewar returns to the lab

In Finland Instruct-FI (Biocenter Finland, coordinated by Butcher, Lehtiö) has submitted a national infrastructure grant proposal aimed at getting a central installation at the CSC for each of the structural biology nodes. This can be extended to other Nordic countries.

Can we get this to work also for other synchrotrons? Can we upload also info on sequence, structure and ligand? Acknowledgements

Ed Daniel (Oulu) Neil Smith, Karl Levik, Alun Ashton (Diamond) Joel Sussman, Orly Dym (Weizmann)

Kristian Koski, Mirko Maksimainen, Lari Lehtiö (Oulu) Protein crystallography community in Oulu (Oulu) Instruct-FI community in Finland (Finland)

Instruct-ULTRA (EU) Diamond (UK)

