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

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This is an
Instruct-ULTRA project

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http://www.oulu.fi/biocenter/protein-crystallography/struct/crystallization/icebear
https://icebear.oulu.fi/help/
https://icebear.oulu.fi/ (user/password: demo/demo; there is on-line help)

The crystallization devices and data collection devices are very expensive

The sample preparation of the protein is usually very demanding

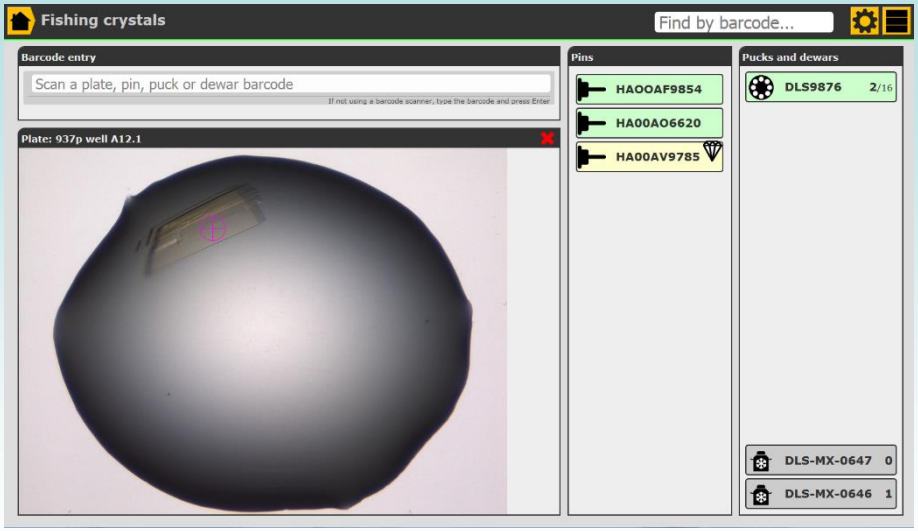
The protein crystallography protocols require much expertise, that students need to learn

Good visualization of crystallization results will foster discussions on these experiments and has educational value

Developing a home-lab data base of the crystallisation results is essential for good research-data-management.

It requires good links to the information concerning the X-ray characterisation from mounted crystals or from in-situ plate scanning

The IceBear development is an Instruct-FI and Instruct-ULTRA project



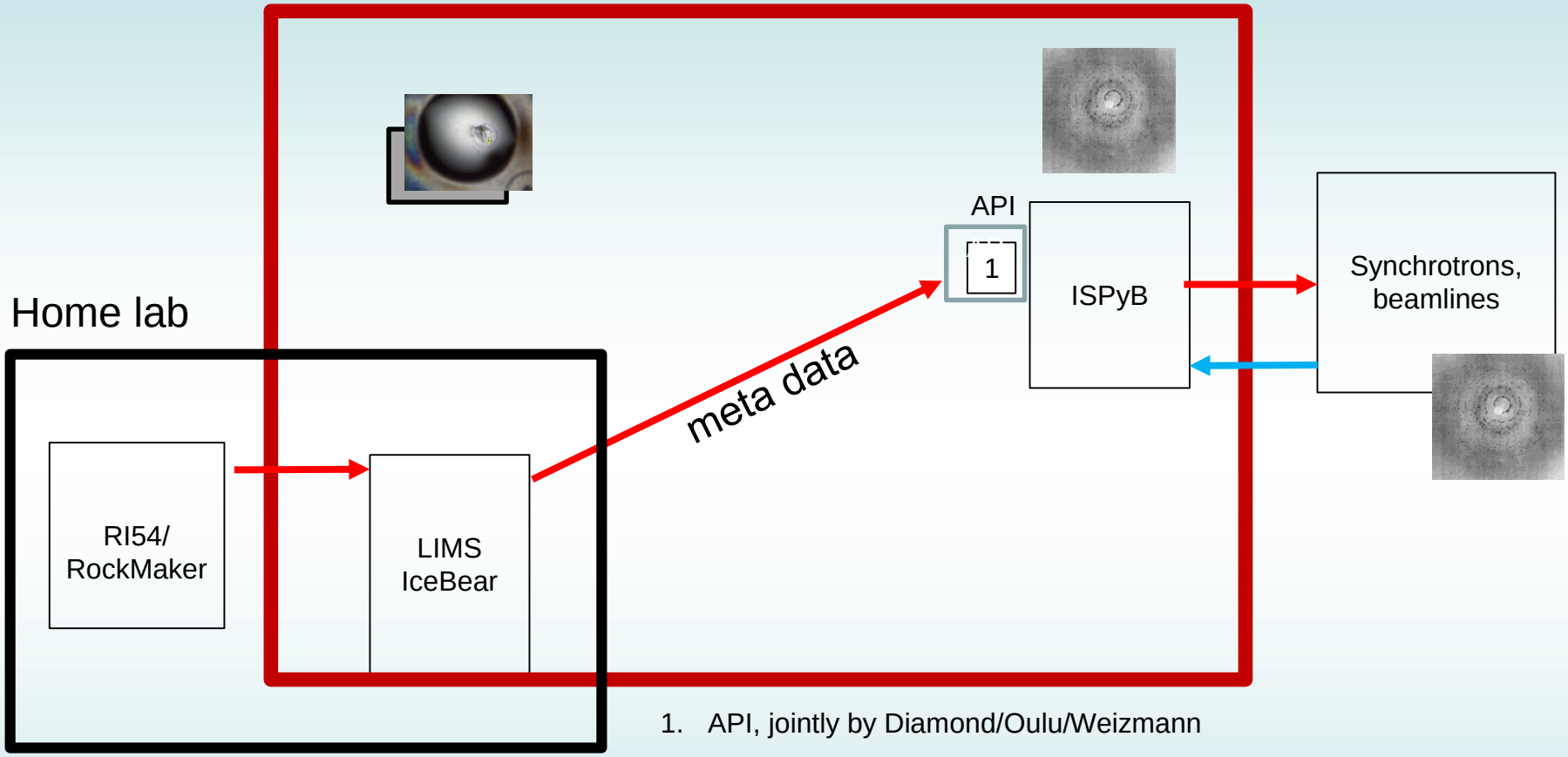
Using IceBear when freezing crystals:

a frozen, harvested crystal gets an identifier (LMTIM_9098A01d1c1), being then associated with a pinbarcode (or a puck position)

Pins can be recycled

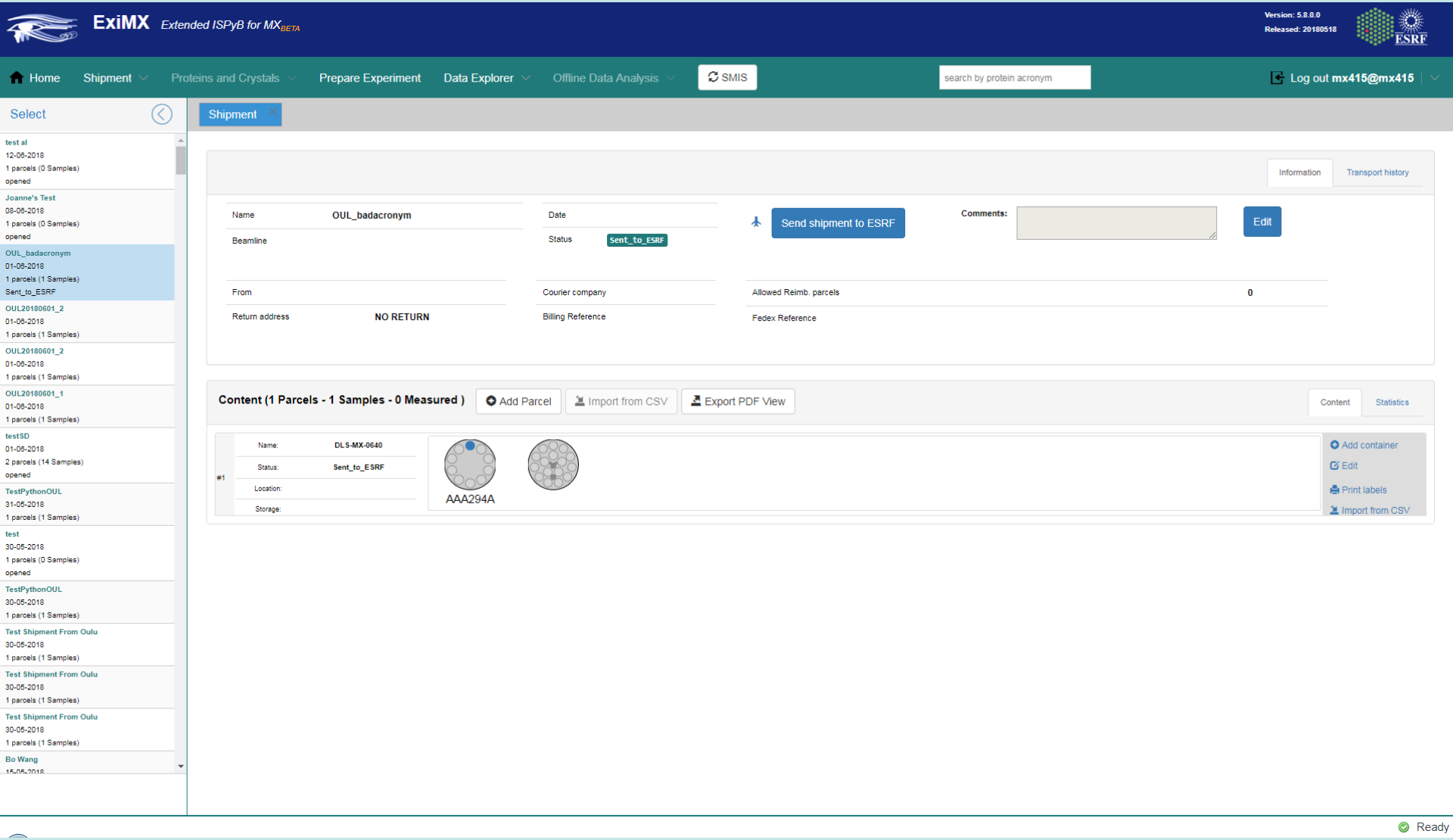
This will also work if a lab does not have a Formulatrix imager

The current IceBear developmental version should be ready for use in Oulu September 2018

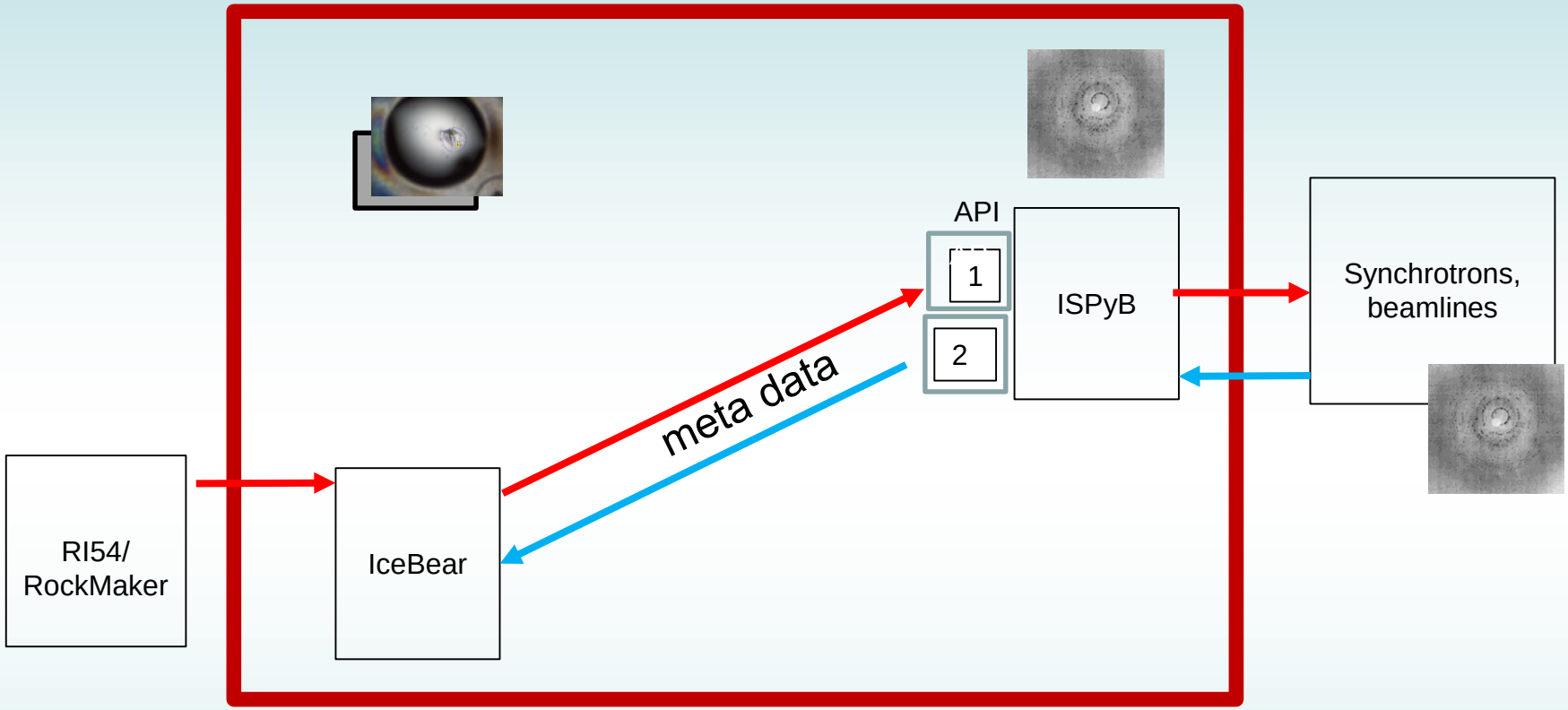


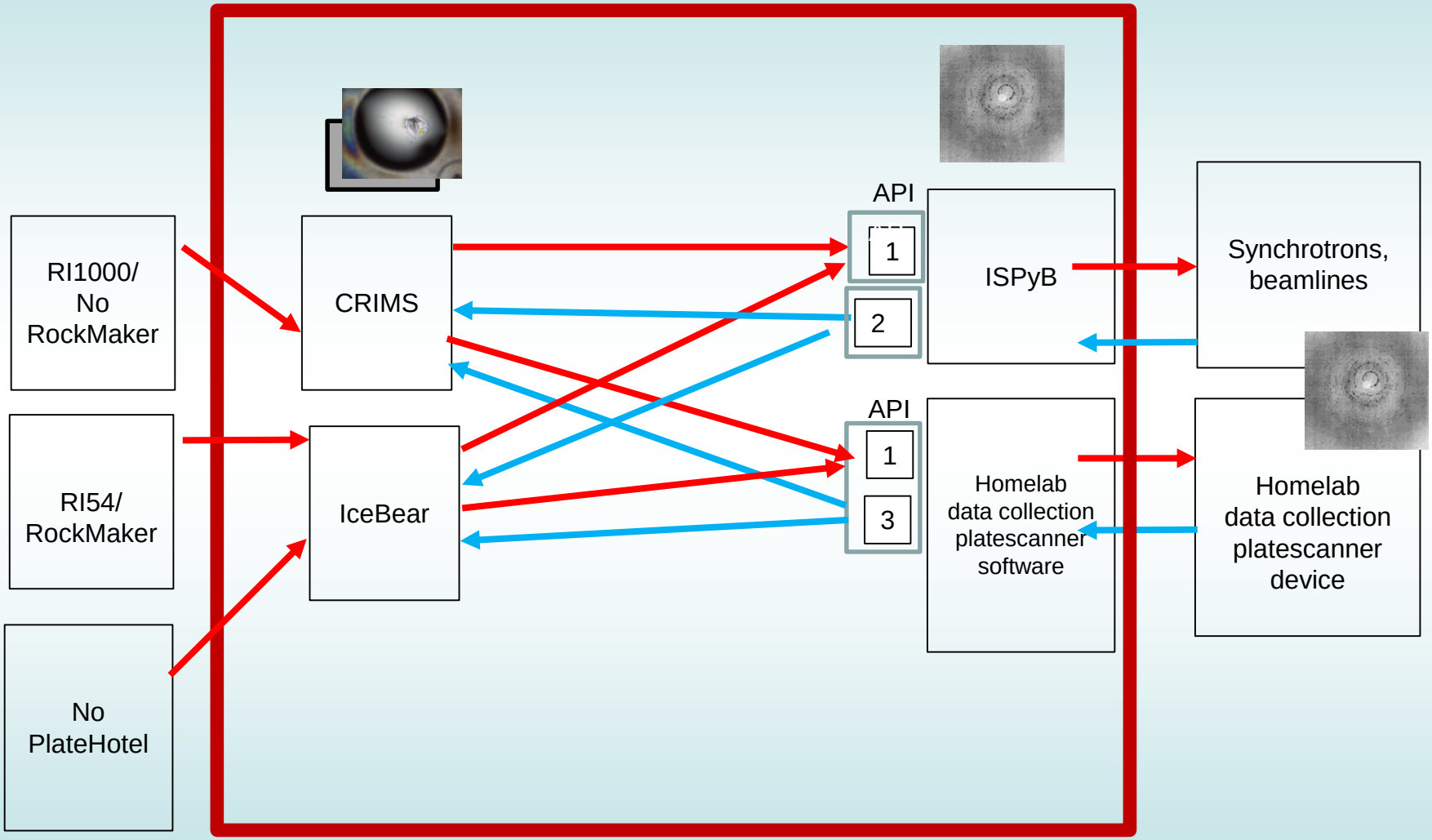
1. API, jointly by Diamond/Oulu/Weizmann

Homelab LIMS: a data base of information on the crystallization results
There are many synchrotrons with different flavors of ISPyB
Delivery of meta-data via an API to ISPyB



Meta data uploaded by IceBear into the ESRF ISPyB


API
1
2
ISPyB
Synchrotrons,
beamlines
meta data
RI54/
RockMaker
IceBear


RI1000/
No
RockMaker
RI54/
RockMaker
No
PlateHotel
CRIMS
IceBear
API
1
2
API
1
3
ISPyB
Homelab
data collection
platescanner
software
Synchrotrons,
beamlines
Homelab
data collection
platescanner
device

Authentification issues:

User-identification: Instruct-FI, CSC, Elixir can help?

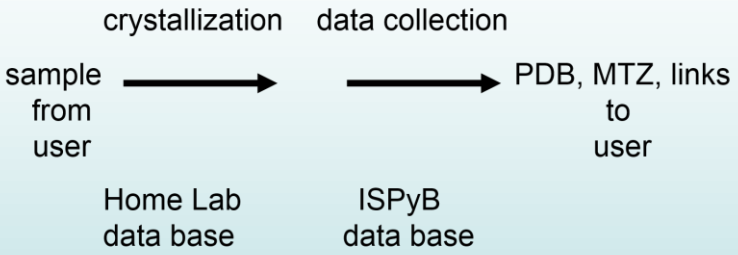
Proposal-identifcation, session identification

Safety-issues: every acronym has to be approved; user-safety-training?

Practicalities:

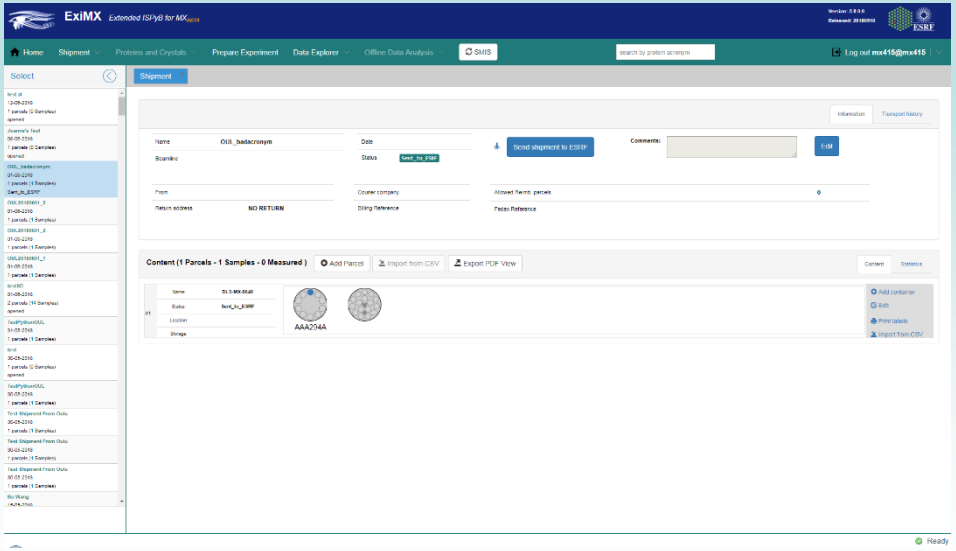
-the homelab needs “shippers” for preparing the shipment and a dewar-recovery-protocol

-Oulu can crystallise for a research group in Sweden, can sent crystals to synchrotron, and then the Swedish group can get the results via ISPyB (needs to be registrated!)



-How about plate scanning?

-What information should homelab sent? What information should it receive?



Actions

-can we set up a time line of actions?
-include the exchange of links
-all data is submitted in one shot (ideally verified before submitting)
-first focus on shipping frozen crystals in pucks and dewars

FROZEN CRYSTAL SHIPMENT

chosen crystals:
-protein acronym
-pin-barcode
-spacegroup/cell dimensions/”OSC-SAD-MAD”/resolution-info
-sequence information
-PDB-code, chain-identifier?
-ligand-code (name, PDB-code, InChl-key)
-URL of crystal selection page
-sample name: crystal-identifier (TIM-9098A1D2C1-“pinbar-code”-“user-part”) -
-identification of the dewar
--position in the puck
--position of puck in the dewar
-drop image?
-remarks

RETRIEVAL OF META DATA

Cross-reference of homelab-LIMS-crystal-identifier (**sender-ID**) and synchrotron-ISPyB-pin/crystal-identifier (**synchrotron-ID**)