



ICAT - ISPyB Meeting

Alba status report

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Computing - MIS

ICAT progress update



- **ICAT Dockerization:** Containerized ICAT applications using Docker.
- **Kubernetes Deployment:** Implemented Kubernetes for automated ICAT deployment.
- **Canary Cookie Approach:** Made Data Portal coexist with Data Hub, with the use of a cookie and canary deployments from K8s ingress controllers.



- **User login:** Users now login using the user portal credentials via Keycloak (Alba SSO).

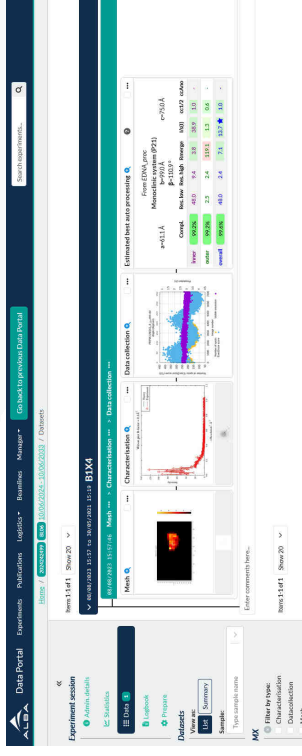
ICAT progress update

- **Ingesting related datasets at same time:** Both raw and processed datasets are ingested when processing data is generated (not automated with MXCube yet).
- **Ingested data:** Recent success on MX data ingestion from pipelines.

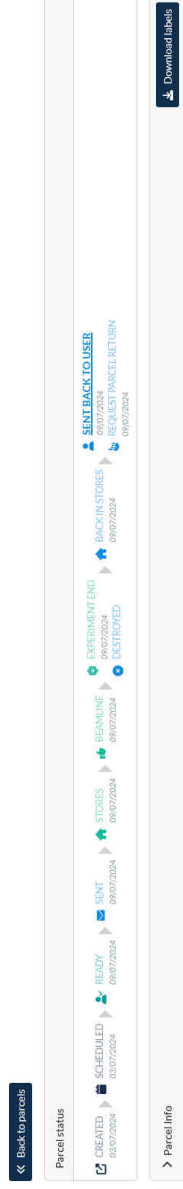
Estimated best auto processing

From *fastrip_anom_run1*
Tetragonal system (P422) *c*-78.6 Å
a-*b*-78.6 Å

	Compl.	Res_low	Res_high	Rmerge	I σ (I)	cc1/2	ccAno
linear	99.1%	27.8	5.9	4.3	51.6	1.0	-
outer	99.6%	1.4	1.3	78.1	2.9	0.8	-
overall	100.0%	27.8	1.3	6.0	19.8	1.0	-

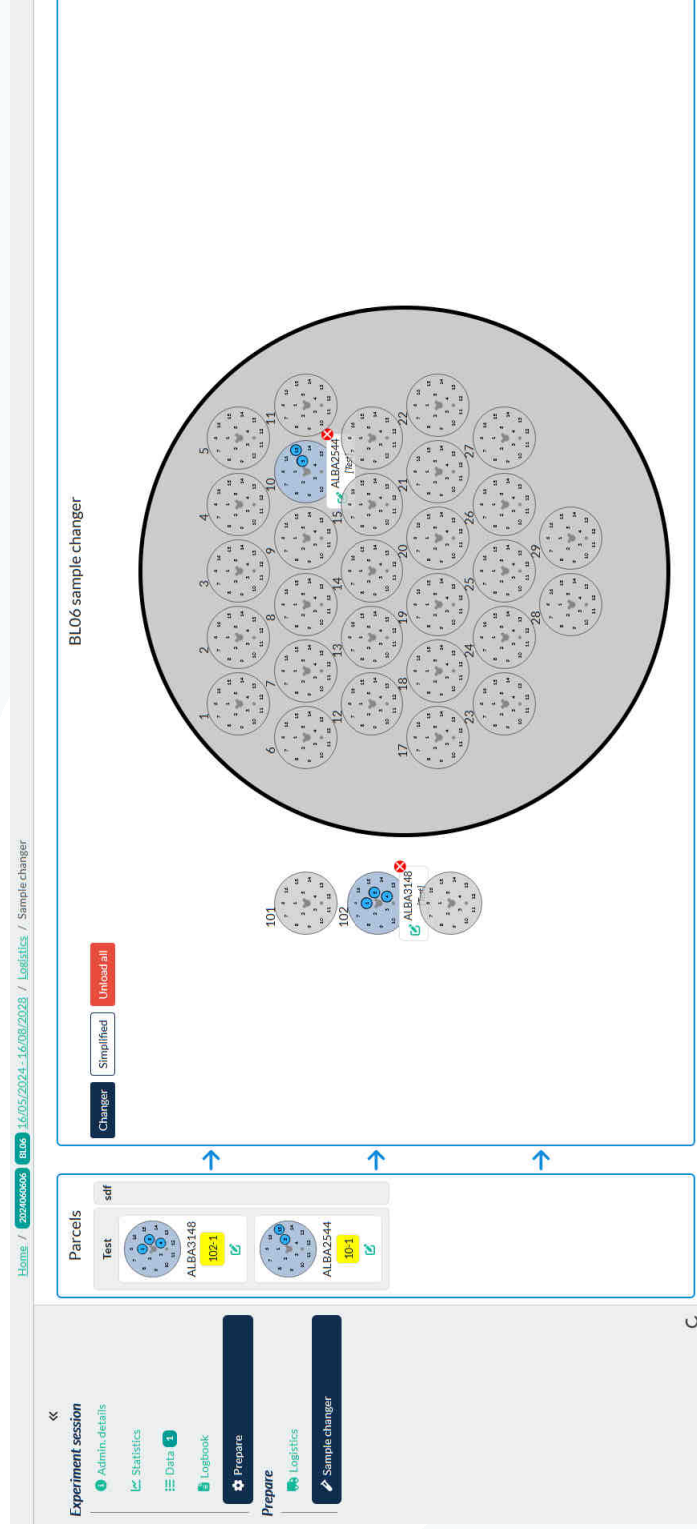


- **Sample tracking:** Workflow for sample tracking/shipping was adapted.



ICAT progress update

- ISARA: Implemented the sample changer in data portal.



The screenshot displays the 'BLO6 sample changer' configuration page in the ICAT data portal. The interface includes a navigation menu on the left with options like 'Experiment session', 'Admin. details', 'Statistics', 'Data', 'Logbook', 'Prepare', and 'Logistics'. The main content area is titled 'BLO6 sample changer' and features a large circular diagram representing the sample changer layout. This diagram is divided into 30 numbered positions (0-29) arranged in a circular pattern. A tooltip for position 13 shows a sample ID 'ALBA3148' with a red 'X' icon. Below the main diagram, there are three smaller circular diagrams labeled 101, 102, and ALBA3148, with the latter also showing a red 'X' icon. On the left side of the main diagram, there are three buttons: 'Changer', 'Simplified', and 'Unload all'. At the top of the page, there is a breadcrumb trail: 'Home / 2024060606 (806) / 16/05/2024-16/08/2028 / Logistics / Sample changer'. The page number '7' is visible in the bottom right corner.

ICAT progress update

- **Beamlines in production:**
 - BL20 - Lorea: Using generic visualizations.
 - BL06 - Xaira: Using MX microfrontend for data visualization.

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Experiment sessions

Search:

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Beamline:

Start date:

Start date:

End date:

User:

Beamline	Start	Title	A-Form	Samples	Datasets	Files	Release	DOI	Logbook
BL20	21/11/2024	Probing Wave Antimagnetism in CrSi					23/11/2027		
BL20	05/11/2024	Electronic structure study of magnetic Kagome material YFe ₆ Ge ₆					10/11/2027		
BL20	30/10/2024	ARPES study on the quasi-symmetry protected gap of CdBiTe		6	958.39 MB	14	04/11/2027		
BL20	28/10/2024	Electronic and magnetic structure studies of Altermagnets					28/10/2027		
BL20	17/10/2024	Parallel spin-momentum locking of multifold fermions in chiral topological semimetals					21/10/2027		
BL20	15/10/2024	The role of the intercalant transition metal in X1/3TbS ₂ (X=Fe, Co)					17/10/2027		
BL20	02/10/2024	Surface band structure engineering of MnBi ₂ Te ₄ family materials for enhanced quantum anomalous Hall effect					04/10/2027		
BL20	25/09/2024	Electronic band splitting and spin texture induced by Dresselhaus spin-orbit coupling in ZnTe					29/09/2027		
BL20	17/09/2024	Flat band Engineering in Co _{0.2} P _{0.8} Ge _{1.02} and Fe ₅ Ge ₁₂		25	7.55 GB	32	23/09/2027	DOI: 10.5777/DALBA-ES-2024028105	
BL20	16/07/2024	Spin and Angle-Resolved photoemission investigations on the spin texture of magnetically modified topological surface states		14	265.58 MB	14	20/07/2027	DOI: 10.5777/DALBA-ES-2024028359	
BL20	10/07/2024	Atomic mechanisms of electron doping in perovskite nickelates		254	3.98 GB	270	14/07/2027	DOI: 10.5777/DALBA-ES-2024028252	
BL06	02/07/2024	First tests for advanced macromolecular cryocrystallography at microfocus beamline XA10A		71	138	24.830	20/11/2027	DOI: 10.5777/DALBA-ES-2024066471	
BL06	01/07/2024	MIS testing		1	171.86 GB	171.86 GB			
BL20	04/06/2024	Inspecting the band structure of ZnAs ₂ , a promising optoelectronic material		187	2.10 GB	262	2/10/2027	DOI: 10.5777/DALBA-ES-2024087678	
BL20	28/05/2024	Correlation between stoichiometry and spin-resolved band structure of manganese telluride monolayers through XPS and (s)-ARPES		162	2.98 GB	187	02/06/2027	DOI: 10.5777/DALBA-ES-2024087382	

ICAT next steps



- **ICAT server components to different Dockerfiles:** Divide ICAT server components into independent Docker containers to improve deployment times.
- **MXCube Integration:** Integrate MXCube with ICAT to automate data ingestion for macromolecular crystallography.
- **Integrate offline pipeline triggering:** We need to decide which tool Will be used and integrate different parameter settings for each available pipeline.
- **Python Ingestor Development:** Python-based ingestor development (to be confirmed).

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- **Notification system:** Taking into account Alba shipping financing program we implemented a notification system to involve Store managers and MRW into the sample tracking workflow.
- **Barcode as link:** Added a barcode containing a direct link to shipment to ease Store managers actions.

The screenshot displays the ExIMX web application interface. The top navigation bar includes 'Home', 'Shipment', 'Prepare Equipment', 'Patterns & Crystals', 'Data Explorer', 'Manager', and 'Help'. The main content area shows a 'Shipment' form with the following details:

- Name:** BSL-2019013247
- Barcode:** BSL2-SALUC
- Date:** 2019-11-20
- State:** Completed
- Shipment number:** [BLSL2019013247-PSF-7](#)
- From:** BSL2-SALUC
- Ship to:** BSL2-SALUC
- Origin:** BSL2-SALUC
- Destination:** BSL2-SALUC
- Weight and measures:** 19112004, 16, 160000, 160

At the bottom, there is a 'Convert (2 Parcels - 0 Measured)' section with a 'PSF-7' label and a 'Print' button.

The screenshot shows a shipping label for 'PSF-7'. It features a large barcode at the top. Below the barcode, the following information is displayed:

- Parcel label:** PSF-7
- Shipment name:** Stef_19Nov2024
- Number of parcels:** 2
- Proposal number:** MX-2019013247
- Laboratory name:** Lilly
- Local contact:** Boer R

ISPyB next steps



- **Improve the notification system:** If keeping long term relationship with MRW we might use their API to automate orders from the applications (to be discussed).
- **Update pucks positions from lab:** When manually placing pucks in the sample changer it would be very convenient to be able to update these positions automatically in the database.

Acknowledgements - Q&A



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