

An introduction to ISPyB

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I19 EH-1 Remote Users Workshop February 2023

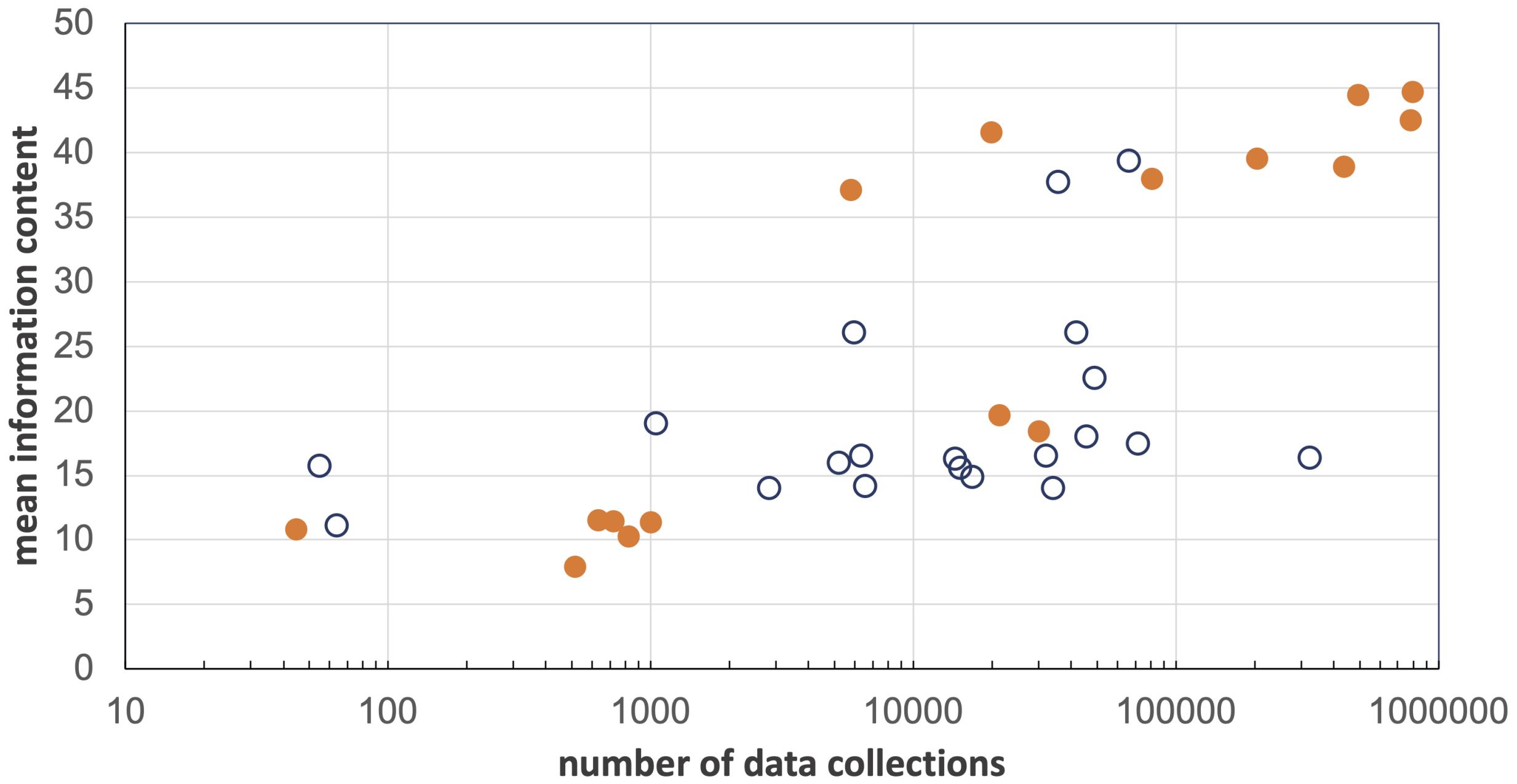


What is ISPyB?

ISPyB is our Laboratory Information Management System

It helps us keep track of:

- Samples
- Data Collections
- Logistics
- and more!



ISPyB is:

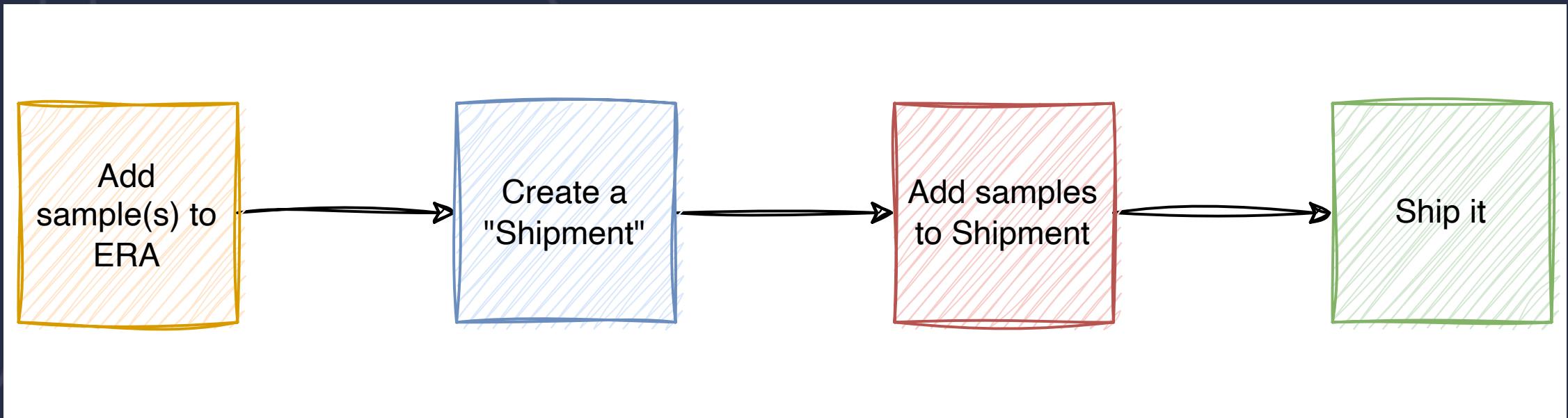
-  a stable, efficient database supporting many beamlines at Diamond

ISPyB is not:

-  specifically made for small molecule crystallography

Before Your Experiment

Process Overview



<https://www.diamond.ac.uk/Instruments/Crystallography/I19/Manual/EH1.html>

Step 1: Add Sample(s) to ERA

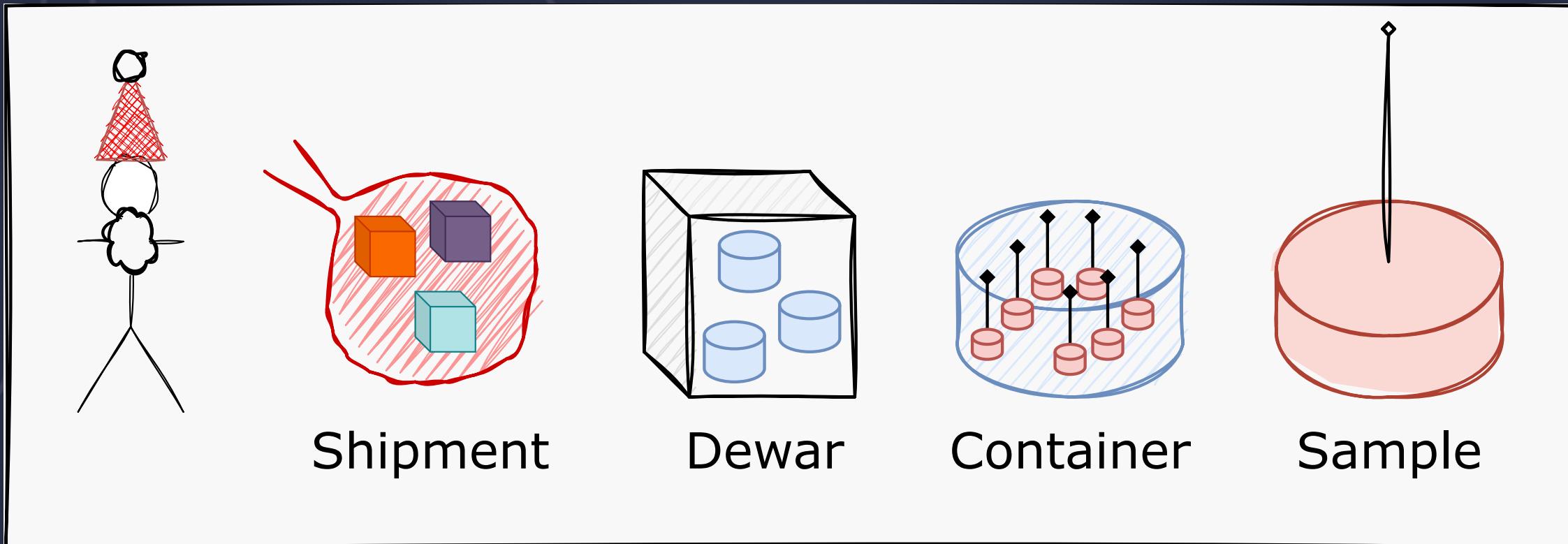
1. uas.diamond.ac.uk
2. Add your samples to the ERA as usual
3. Add an acronym

Sample Material or Protein
cytidine

Acronym
cyt

- Step 1a: Wait for ERA to be validated
- Step 1b: Wait for 10 minutes past the next hour
- Step 1c: Wait for another 20 minutes

A couple of definitions



Step 2: Create the Shipment

1. ispyb.diamond.ac.uk
2. Log in and find the relevant proposal
3. Create a *Lab Contact*

| Proposals | cm26454 ▾ | Projects |
|--------------------------------------|-----------------------|------------------------------|
| The start of run 5 has been delayed. | View All Data | day 19th November. |
| | Visits | |
| | Calendar | |
| | Assign Containers | |
| | Shipments | |
| | Registered Dewars | |
| | Registered Containers | Dr Sarah Barnett, Dr Sarah |
| | Containers | sarah Barnett, Dr Dave Allan |
| | Samples | sarah Barnett, Dr Sarah Barn |
| | Proteins | |
| | Lab Contacts | |
| | Statistics | sarah Barnett, Dr Sarah Barn |
| | Migrate | |

Visit List

This page lists the visits available to

| Start | End | Nu |
|---------------------|---------------------|----|
| 09:00 23-10-2020 | 09:00 31-12-2020 | |
| 09:00 14-08-2020 | 09:00 23-10-2020 | |
| 09:00 22-05-2020 | 09:00 14-08-2020 | |
| 09:00 06-03-2020 | 09:00 22-05-2020 | |
| 13:50 06-01-2020 | 13:50 06-01-2020 | |
| 09:00 01-01-2020 | 09:00 06-03-2020 | |

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2a: Create a lab contact

The lab contact is the name and address of the person sending the samples to Diamond



Add New Home Lab Contact

Card Name
Name for the Contact Card Choose something that will be easily recognisable,
e.g., your name, in the list of contacts

Contact Details

Contact Family Name
The person's family name

Contact First Name
The person's first name

Contact Phone Number
The person's phone number

Contact Email
The person's email address

Contact Laboratory Details

Laboratory Name
The contact's laboratory name

Laboratory Street Address
Street Address (excluding post code, city)
There is a line limit of 35 characters so add over multiple lines where necessary

Only include address lines which are not required specifically elsewhere

Laboratory City
The contact's laboratory city

Laboratory Postcode
The contact's laboratory postcode

Laboratory Country
The contact's laboratory country United Kingdom

Dewar Return Details The following information is used for each shipment associated with this contact

Courier Company
Courier company to use to return dewars to home lab

This section should be left blank
if using the Diamond Courier
(only available for UK addresses)

Courier Account No.
Courier account number for returning dewars to home
lab

Billing Reference
Billing reference to use when returning dewars to home
lab

Average customs value of dewar
The average customs value of a dewar

Average transport value of dewar
The average transport value of a dewar

Add Home Lab Contact

Click here to add the contact, or save changes, once done

2a: Create a lab contact

The lab contact is the name and address of the person sending the samples to Diamond



2b: Register Dewars

Dewars need to be registered in the database to be usable. DLS-owned Dewars will already have been registered and so will have an identifier of the form

DLS-CY-00XX

If you are using your own Dewar, you will need to register it yourself



2c: Create Shipment

Shipments

This page shows a list of shipments associated with the currently selected proposal

In order to register your samples you need to create a shipment. Shipments contain dewars, dewars contain containers, and containers individual samples. These can be created sequentially by viewing a particular shipment

+ Add Shipment

| Name | Creation Date | Outgoing Contact | Return Contact | Status | # Comp | Comments |
|---------------|---------------|------------------|----------------|--------|--------|----------|
| Sarah Barnett | 18-06-2020 | Sarah Barnett | Sarah Barnett | opened | 2 | |

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Step 3: Add Samples to Shipment

You've created a Shipment. Now lets add some samples to it



3a: Create Container

Shipment Contents

Select a dewar by clicking on the row in the table below. Dewar details are then shown below. Click the + icon to add a container to the selected dewar

+ Add Dewar

| Name | Barcode | Facility Code | Weight (Kg) | First Experiment | Tracking # to | Tracking # from | Status | Location | Containers | Actions |
|------|-------------------------|---------------|-------------|------------------|---------------|-----------------|--------|----------|------------|---------|
| Test | cm26454-5-i19-1-0044018 | DLS-CY-0002 | 18 | cm26454-5 | Click to edit | Click to edit | opened | | 0 | |

Dewar Details: **Test**

+ Add Container

This section shows contents and history for the selected dewar. Click the spyglass icon to view the contents of the container

No Containers for this dewar

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| Date | Status | Location |
|----------------------|--------|----------|
| No history available | | |

15 ▾ Page < (1) >

Origin N/A
Destination N/A

| Date | Status | Location | Signatory |
|-----------------------|--------|----------|-----------|
| No tracking available | | | |

Container: I19-0064

This page shows the contents of the selected container. Samples can be added and edited by clicking the pencil icon, and removed by clicking the x

| Shipment | Test | | | | | | | | |
|----------------------|---|----------|------------|----------|----------|------------------|--------------|--------|---|
| Dewar | Test | | | | | | | | |
| Container Type | Puck | | | | | | | | |
| Registered Container | Click to edit | | | | | | | | |
| Barcode | Click to edit | | | | | | | | |
| Priority Processing | xia2/DIALS | | | | | | | | |
| Automated Collection | + Queue this container for Auto Collect | | | | | | | | |
| Comments | Click to edit | | | | | | | | |
| Location History | <table><thead><tr><th>Date</th><th>Status</th><th>Location</th><th>Beamline</th></tr></thead><tbody><tr><td colspan="4">No history found</td></tr></tbody></table> <p>10 Page « ‹ 1 › »</p> | Date | Status | Location | Beamline | No history found | | | |
| Date | Status | Location | Beamline | | | | | | |
| No history found | | | | | | | | | |
| Location | Protein Acronym | Name | Spacegroup | Barcode | Comment | Anomalous | Required Res | Status | + Extra Fields |
| 1 | cyt | C1 | | | | | | | |
| 2 | cyt | | | | | | | | |
| 3 | Fru | F1 | | | | | | | |
| 4 | <input checked="" type="checkbox"/> cyt | | | | | | | | |
| 4 | <input checked="" type="checkbox"/> Fru | S1 | | | | | | | |
| 5 | <input checked="" type="checkbox"/> Suc | | | | | | | | |

3b: Put samples in Container

1. Dewar Tracking Label



diamond



* c m 2 6 4 5 4 - 5 - i 1 9 - 1 - 0 0 4 4 0 1 8 *

| | |
|---------------|----------------------|
| Label | Test |
| Shipping Name | Test |
| Safety Level | Green |
| No. Parcels | 1 |
| Proposal | cm26454 |
| Home Lab Name | Diamond Light Source |
| Local Contact | Dr Sarah Barnett, |

1. Print the labels out
2. Stick them to your Dewar



3. Ship it



During Your Experiment

During the visit you can see what's going on

The screenshot shows a web browser window for the ISPyB Data Collections interface. The URL is <https://ispyb.diamond.ac.uk/dc/visit/cm33867-1>. The page title is "Data Collections for cm33867-1 on i19-1". A navigation bar at the top includes links for Assign Containers, Summary, Auto Processing, Visit Stats, Users, Dewars, Sample Changer, Reprocessing, and Beamline Status.

The main content area is titled "i19-1 Webcams & Beamline Status". It displays various status indicators in colored boxes:

- Ring Current: 299.853 (green)
- Refill: 289.727 (green)
- Hutch Locked (green)
- Port Shutter Open (green)
- Fast Shutter Closed (red)
- Energy: 25.4926 (green)
- Current Puck: 0 (green)
- Current Pin: 0 (green)

Below these are two green sections labeled "Machine Status 1" and "Machine Status 2".

At the bottom, there are two video thumbnails showing beamline equipment. The left thumbnail is dated 2023-02-05 18:45:19 and shows a close-up of a metal pipe and a circular opening. The right thumbnail is also dated 2023-02-05 18:45:19 and shows a wider view of the beamline with several white circular components.

The Data Collections Page

2023-02-01 10:02:05 - rebecca_01022023/screenings/01_NiI2|ut4_100K/NiI2|ut4_01 #####.cbf

| | |
|-------------------------------|----------------------|
| Flux: | Φ Start: 0.0° |
| Φ Osc: 0.10° | Φ Overlap: 0° |
| No. Images: 450 | ω : 0° |
| Resolution: 0.96 Å | Wavelength: 0.6889 Å |
| Detector Distance: 160.0mm | Detector 2θ: 0 |
| Transmission: 0.01% | Exposure: 0.1000s |
| Type: Screening | Beamsize: 0x0 μm |

Comment:

Auto Processing xia2 dials-aimless ✓ xia2 dials ✓

Downstream Processing

The concept of a data collection group



the reciprocal lattice viewer







A scatter plot showing a large number of teal-colored data points forming a roughly triangular shape. Two thick, intersecting lines are overlaid on the plot: a light green line sloping down from left to right, and a light red line sloping up from left to right. They intersect at approximately the center of the data cluster. In the bottom-left corner, the text "Press h for help" is displayed in a white, sans-serif font.
Press h for help

Processing Summary



Dials / Processing output

Auto Processing

xia2 dials-aimless ✓ xia2 dials ✓

| Type | Resolution | Spacegroup | Mn< sig(i) > | Rmeas Inner | Rmeas Outer | Completeness | Cell | Status |
|--------------------|-------------|------------|--------------|-------------|-------------|--------------|------------------------------------|-----------------------|
| xia2 dials-aimless | 7.68 - 0.82 | P 4/n n c | 7.0 | 0.096 | 1.581 | 93.9 | 12.02 12.02 9.98 90.00 90.00 90.00 | processing successful |
| xia2 dials | 8.50 - 0.82 | P 4/m m m | 11.2 | 0.080 | 1.578 | 76.8 | 12.02 12.02 9.98 90.00 90.00 90.00 | processing successful |

xia2 dials-aimless xia2 dials

| Space Group | A | B | C | α | β | γ | Plots | Archive | Logs & Files | Lookup Cell |
|-------------|-------|-------|------|----------|---------|----------|-------|---------|--------------|-------------|
| P 4/n n c | 12.02 | 12.02 | 9.98 | 90.00 | 90.00 | 90.00 | | | | |

| Shell | Observations | Unique | Resolution | Rmeas | I/sig(I) | CC Half | Completeness | Multiplicity | Anom Completeness | Anom Multiplicity | CC Anom |
|------------|--------------|--------|-------------|-------|----------|---------|--------------|--------------|-------------------|-------------------|---------|
| outerShell | 9 | 8 | 0.82 - 0.84 | 1.581 | 3.5 | 0.0 | 22.9 | 1.1 | 0.0 | 0.0 | 0.0 |
| innerShell | 113 | 47 | 2.22 - 7.68 | 0.096 | 10.3 | 1.0 | 100.0 | 2.4 | 0.0 | 0.0 | 0.0 |
| overall | 1526 | 643 | 0.82 - 7.68 | 0.083 | 7.0 | 1.0 | 93.9 | 2.4 | 0.0 | 0.0 | 0.0 |

Downstream Processing

Live Demo Time!



Imminent Improvements

There are some improvements coming soon which should hopefully make ispyb even more useful 

- Use the supplied formula in shelxt solve
- Attach shelxt outputs correctly as processing outputs

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