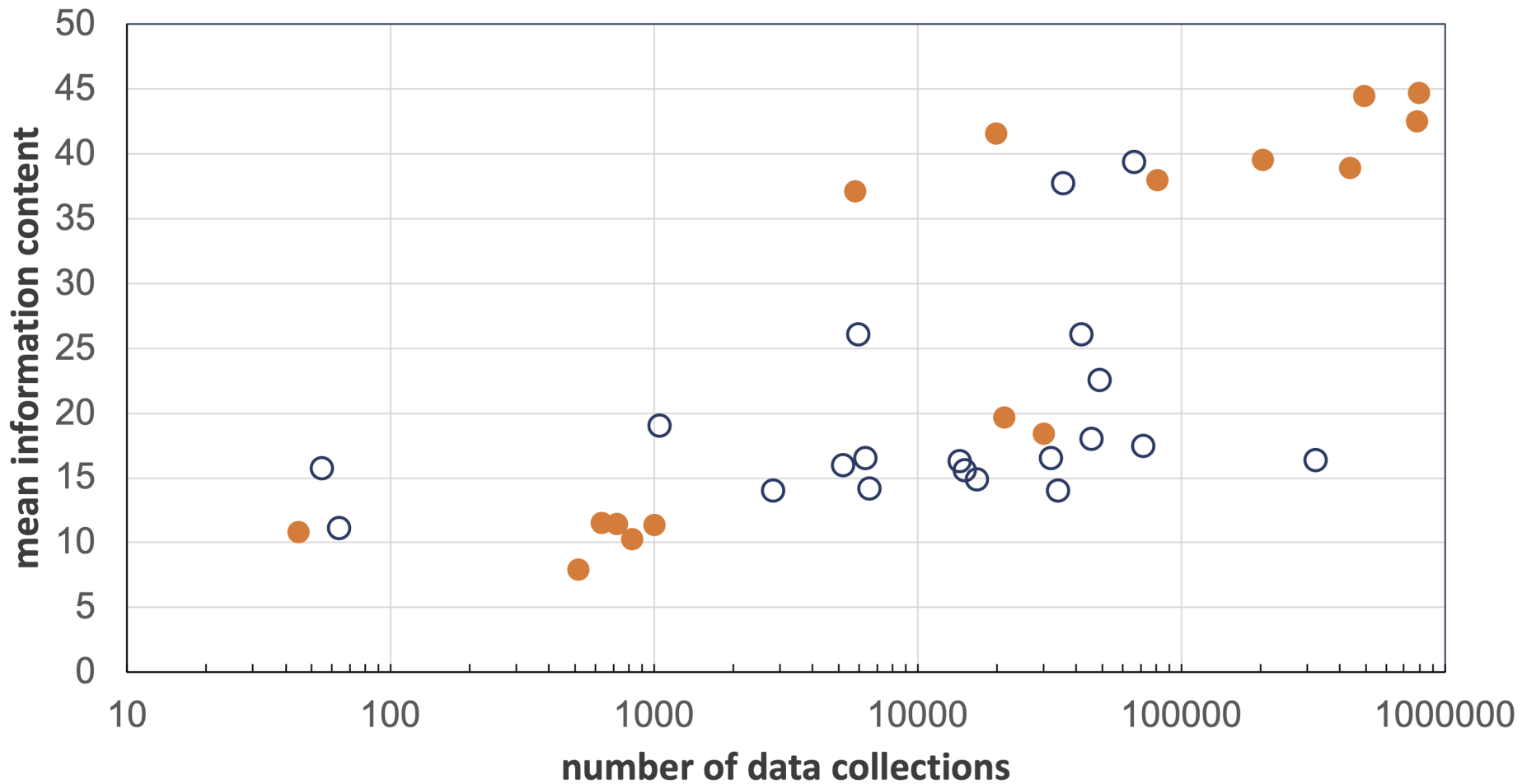


An introduction to ISPyB

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I19 EH-1 Remote Users Workshop February 2023

What is ISPyB and why do we need it?



And that's just the data collection

- What *is* this sample?
- Where did it come from?
- Whose is it?
- What did the results look like?

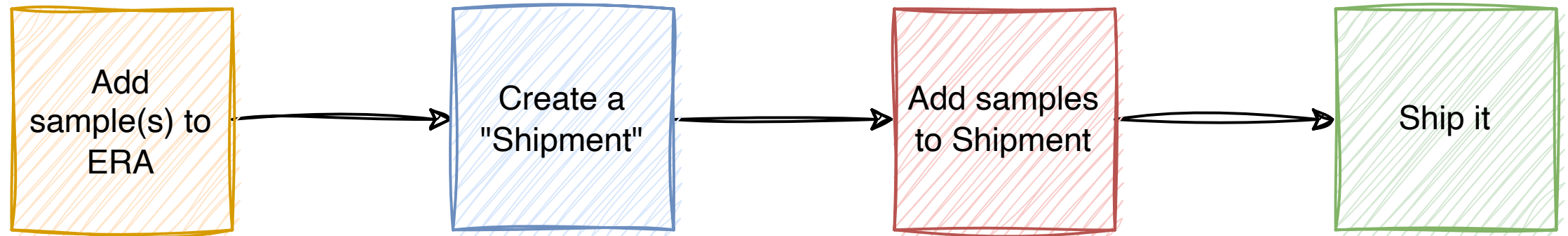
ISPyB is:

✓ a stable, efficient database supporting many beamlines at Diamond

ISPyB is not:

○ specifically made for small molecule crystallography

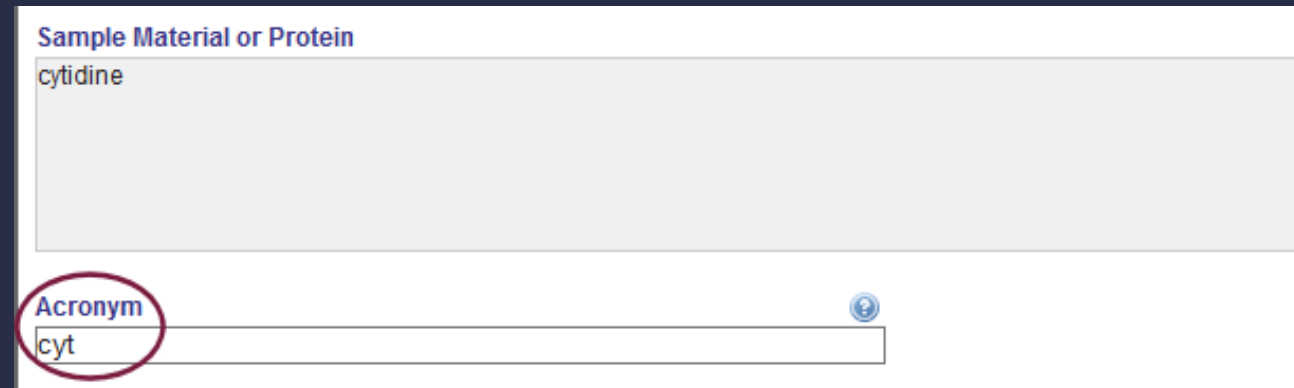
Process Overview



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

Step 1: Add Sample(s) to ERA

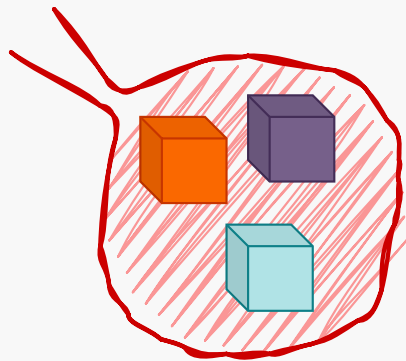
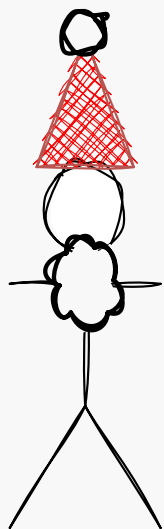
1. uas.diamond.ac.uk
2. Add your samples to the ERA as usual
3. Add an acronym



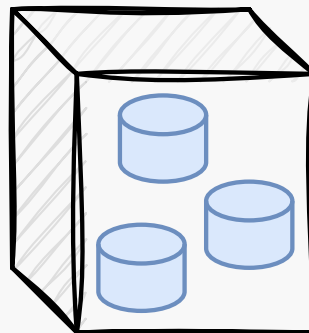
The screenshot shows a web form with two input fields. The first field, titled "Sample Material or Protein", contains the text "cytidine". The second field, titled "Acronym", contains the text "cyt". The "Acronym" label and its input field are circled in red. A small blue question mark icon is located to the right of the "Acronym" field.

Step 1a: Wait for ERA to be validated
(...and then 3 hours more)

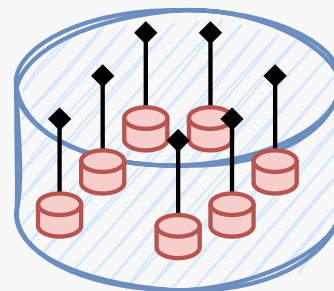
A couple of definitions



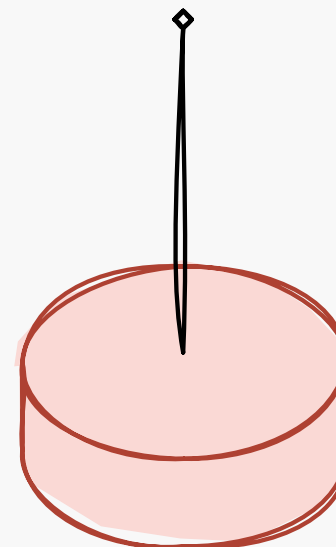
Shipment



Dewar



Container



Sample

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	
Visit List	Calendar	
This page lists the visits available to	Assign Containers	
	Shipments	
	Registered Dewars	
	Registered Containers	Dr Sarah Barnett, Dr Sarah
	Containers	arah Barnett, Dr Dave Allan
	Samples	arah Barnett, Dr Sarah Barr
	Proteins	
	Lab Contacts	
	Statistics	arah Barnett, Dr Sarah Barr
	Migrate	

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

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

Dewar Return Details

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

Courier Company This section should be left blank
Courier company to use to return dewars to home lab 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

2c: Create Shipment

Step 3: Add Samples to Shipment

3a: Create Container

3b: Put samples in Container



Ship it

Using ISPyB during your experiment

During the visit you can see what's going on

ISPyB » Data Collections » i19-1 X

https://ispyb.diamond.ac.uk/dc/visit/cm33867-1

For quick access, place your bookmarks here on the bookmarks toolbar. [Manage bookmarks...](#) Other Bookmarks

Data Collections for cm33867-1 on i19-1

[Assign Containers](#) [Summary](#) [Auto Processing](#) [Visit Stats](#) [Users](#) [Dewars](#) [Sample Changer](#) [Reprocessing](#) [Beamline Status](#)


i19-1 Webcams & Beamline Status

Ring Current 299.853	Refill 289.727	Hutch Locked	Port Shutter Open	Fast Shutter Closed	Energy 25.4926	Current Puck 0	Current Pin 0
ID Gap 5.25995							

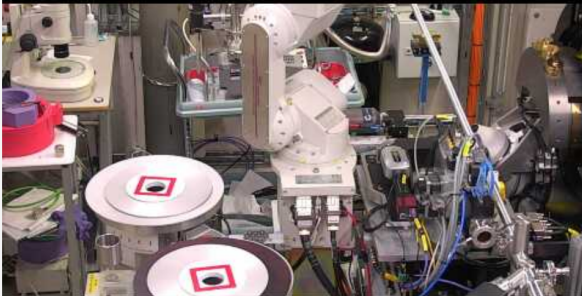
Machine Status 1
User beam time

Machine Status 2

2023-02-05 18:45:19



2023-02-05 18:45:19



Data Collections Page, the distl plot

The concept of a data collection group

the reciprocal lattice viewer

Processing Summary

Processing Outputs

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