Status ISPyB @ESRF

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Roadmap achieved for last 4 years

- Following what was agreed in the ISPyB Strategy Meeting @Hamburg **2020**

ISPyB

SynchWeb

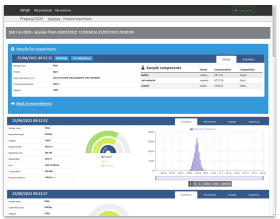
Development framework
Authenticators
UO synch…

GitHub

FastAPI

python

Develop SSX
Frontend/backend
MxCube…



SSX UI

Evaluation

January 2023

Development + Migration

py-ispyb

Main contributors: EMBL DESY. ESRF The European Synchrotron

Evaluation of py-ispyb

- **py-ispyb**
  - …**updates** the ISPyB software stack (python, FastAPI, SQLAlchemy…)
  - …removes unused **legacy** features accumulated over the years
  - …**makes** work **easier** thanks to a modern framework (auto-generated code)
  - etc…

- **…BUT**
  - did not decrease the **complexity** (>210 tables)
  - New techniques implies changes in the **data model + web services + UI**
    - Example:
      - SSX data model (+ 7 tables)
      - Web services read/write
  - It **lacks flexibility** in how entities are linked. (Data collection, DCG, Sample, etc…)
    - Merging data from multiple sessions, samples, etc…
  - did **not** dramatically improve **collaboration** due to little commitment from partners
  - It does not manage raw data
  - It is not compliant with the data policy
  - etc…

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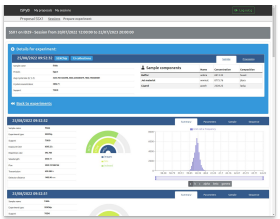

SSX UI

Evaluation

ICAT

Development
+
Migration

WE ARE HERE

Evaluation

Main contributors: EMBL DESY. ESRF The European Synchrotron

Who uses what

Technique	Backend	UI
MX	ISPyB	py-ispyb-ui
		EXI
	ICAT*	Data Portal*
BioSAXS	ISPyB	EXI
	ICAT*	Data Portal*
EM-SP	ISPyB	py-ispyb-ui
EM-ET	ICAT*	Data Portal*
SSX	py-ispyb	py-ispyb-ui

Discontinued

* Under testing

Main contributors: EMBL

ESRF
The European Synchrotron

Currently

- Continue porting existing ISPyB features to ICAT
  - Phasing/MR
  - Characterisation metadata

- Add/improve missing features that were not developed in ISPyB
  - Reprocessing
  - Merging of datasets
  - Working closely with scientists to define better visualization

- Extending ICAT's based solution to other beamlines
  - All beamlines are plugged into ICAT for RAW data
  - Only two beamlines are pushing processed results

- Keeping both ISPyB running in parallel
  - Continue testing and comparing both approaches