

# 1<sup>st</sup> ISPyB Collaborative meeting

Hosted by ESRF on 16-18/01/17 together with 10<sup>th</sup> MXCuBE meeting

**presents:** ESRF, CELLS, DLS, HZB, MAXIV, GP, EMBL,

**Documents to provide:** talks, photos, annex2 of contract

1. Collaboration contract almost signed by all collaborators involved, the rest is on-going.
2. Everyone agrees that the hosting site takes note on actions/decisions and distribute it together with the slides presented.
3. List of each committee member is defined in annex2 and validated by STC.
4. **BiOSAXS working group:** (EMBLHH, CELLS, ESRF, SOLEIL, MAXIV, GP?)
  - sites who use ISPYB BIOSAXS today (other don't have a BIOSAXS beamline (ALBA, MAXIV) or don't use it DLS):SOLEIL, ESRF, EMBL HH
  - Identification of areas for collaboration with BIOSAXS ISPYB members based on different wish lists:
    - EXI BIOSAXS fully on-line for users : ESRF-SOLEIL
    - ESRF to end of Jan : add 2 missing elements present in ISPYB (ab initio model, add experiment)
    - ESRF : add shipment creation/description (refurbishing in view of generic usage at ESRF)
    - ESRF : add shipment creation/description (refurbishing in view of generic usage at ESRF)
    - SOLEIL: service opened to friendly users for 6 months, different rules for BAGs (see presentation in ISPYB update session), wish to extend to tomography and "ptychography"???
    - SOLEIL & ESRF : Validation of EXI BIOSAXS and share of developments for small bug fixes, improvements
    - SOLEIL -EMBLHH : Automated SAXS pipeline for membrane proteins integrated into ISPYB WP5 of iNEXT project - deliverable D5.5 due in about 2y - ESRF will be part of the discussions
    - EMBLHH : provides a list of identified modifications
    - ALL 3 sites : refine and define roadmap with work assigned (mainly to SOLEIL)
    - Off-line analysis: ESRF-SOLEIL
      - SOLEIL: provides specifications
      - SOLEIL-ESRF : defines roadmap and split work
5. **Dev meeting:**
  - CryoEM

ISPyB monitor

A lot of Datacollection fields have been added to fit the CryoEM need.

- XPDF

The MX tables (Protein, Crystal, BLSample, BLSampleGroup) have been reused to fit the need of XPDF, but it may lead to problems because it lacks some meaning ( ex: Proteins -> phases)

As it may be a problem to reuse tables used for MX to force them to fit to other techniques (“hijacking”), we shall better work with scientists and developers to define if better extend tables or create new tables.

Ask MX people when changing field for other techniques.

- Generic sample tracking at ESRF

Some fields from Shipping/Dewar/Container/Protein tables will be reused, some will be added.

Later the names of the tables should be modified, or merged with the new “Component” tables added by DLS

- How to deal with the growing DataCollection table ?

Add all fields if concerning collections

- a) Having 2 letters prefix for specific techniques, and keep all in a unique table ?
- b) Split the table, having a core for datacollection and specific tables linked by foreign keys ? easy to add new parameters

To decide if b) could be a good solution:

- 1) A benchmarking has to be done to see how easy and fast it would be to retrieve all dataCollections parameters in several tables linked by foreign keys

-> ESRF

- 2) Fill the datacollection tables with split options -> DLS
- 3) Discuss -> have a meeting dev in 2 to 3 months ?

- Foreign keys ?

Waiting for STC

- Others

Use DB changes tracking

Link between autoprocessing and ISPyB

Raise the issue : document

--> Olof will write documentation about what exists

Write a nexus file to ISPyB converter :

→ DLS will write it

Go to Github

→ ESRF

Docker

→ ESRF

ISPyB packaged with MySQL db, webservice to fill data from User Portal data

Synchweb

→ DLS will put on Github a docker with all

- CryoEM :

Single particle

Adapt CryoEM in ESRF from DLS : medium -> months

SCIPION + SCIPION librairies + python code server

- Steering committee

Next meetings:

June 2017 SOLEIL

December 2017 GP

June 2018 Desy

December 2018 DLS

-> Merge the datamodel :

Add all DLS tables as they are in January 2017 and start from this

-> Use github

-> New proposal goes through science committee and after developers committee