## Future needs for home lab LIMS and ISPyB communications

- Biocenter Oulu Structural Biology core facility
- Instruct-ERIC Centre Finland node
- 10-15 local research groups, 60-70 users
- Teaching at the Faculty of Biochemistry and Molecular Medicine
- Coordinate synchrotron access through national BAGs

ISPyB meeting

Lari Lehtiö

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Development of IceBear was initiated at 2010 to cover our and users needs in crystal data tracking.

BIOCENTER OULU
UNIVERSITY OF OULU

UNIVERSITY OF OULU

FINStruct

instruct ERIC
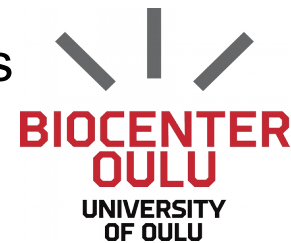
**No-typing crystal shipments**

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Suitable for small home-labs, but also for core facilities:
- Easy to install
- Educational tool
- Easy to communicate between project members
- Works off-campus
- Pin-puck-dewar management
- Works with several imagers
  → Now also crystal shipment module implemented!

# USER NEEDS

1. When solving/refining a crystal structure it is highly relevant to have easy access to ISPyB/raw data as well as to the crystallization/crystal treatment information. This may be years after the experiments and needed by a new team member. *Is it possibly to find the data collection and crystallization details afterwards?*

2. Funding agencies require scientist to describe research data management and home university/institute should establish practices for archiving raw data. *Can we find out retrospectively exactly what was done when preparing the samples?*

3. Increasing amount of samples are shipped to measurements on different synchrotrons. Resulting in lots of data in ISPyB. How to keep track easily? Avoid typing things here and there and? Possible to click and find the relevant data retrospectively?

4. It would be nice if things would "just work". A small individual scientist vs a large infra – no time/skills to maintain computational systems. Wouldn't it be nice to just point your browser somewhere and start working?

# SOFTWARE COMMUNICATION NEEDS

- Compatible with multiple LIMS, not only IceBear/CRIMS
- IceBear, ISPyB data base should be available permanently (persistent links/sample ids)
- Can we use existing APIs to upload sequence, reference structure and ligand information?
- Link from ISPyB sample/shipment to the home LIMS crystal page
- Interoperability allowing building of workflows
- Communication with all European synchrotrons
- IceBear to cloud [EOSC-Life proposal submitted today]
- Other features?

# HOW TO MAKE IT POSSIBLE?

**Uniform API**
- No need to reinvent the wheel for every synchrotron
- General API
    - ideally one shot
    - ligand, sequence, structure info, crystallization info
- Need to be validated for compatibility with the beam line software at each synchrotron at the time of shipment submission

**All European synchrotrons**
**DLS**  - Neil Smith, Dave Hall
**MAXIV** - Alberto Nardella, Jie Nan, Marjolein Thunnissen
**ESRF** - Gianluca Santoni, Alex de Maria
**Others** - ?