



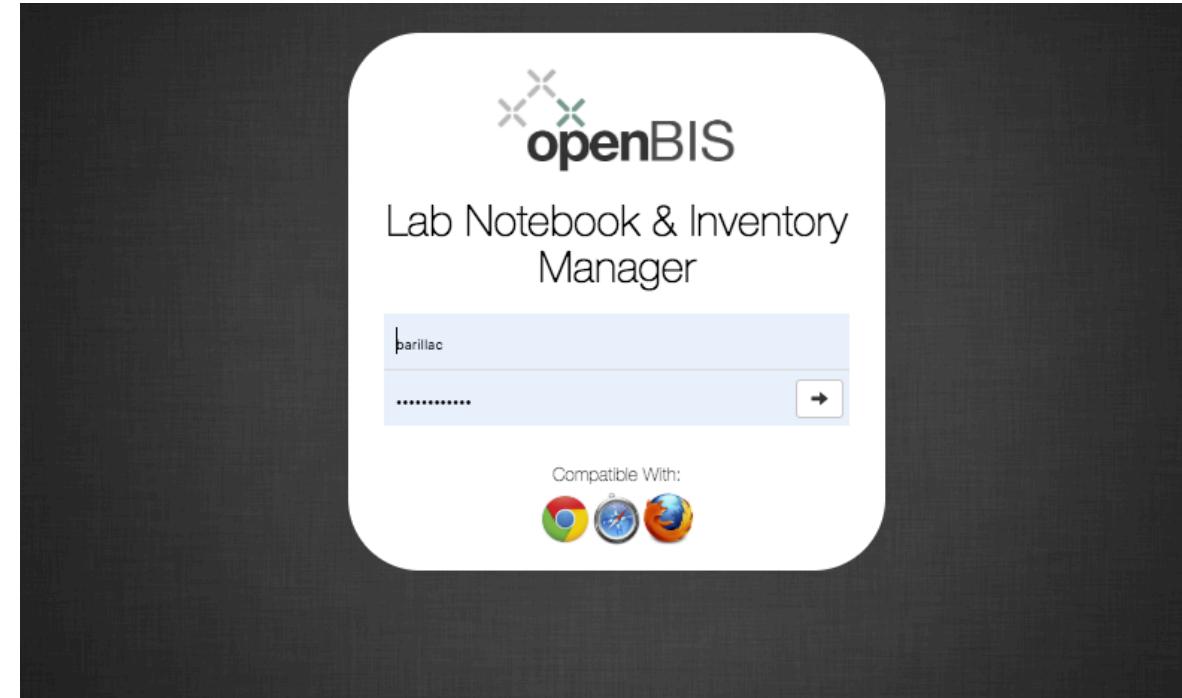
openBIS Training

Caterina Barillari, Priyasma Bhoumik, Henry Lütcke

Scientific IT Services, ETH Zurich

SIB course, 06.05.2020

<https://openbis-training.ethz.ch/openbis/webapp/eln-lims/?>



Course material

<https://edu.sib.swiss/course/view.php?id=452>

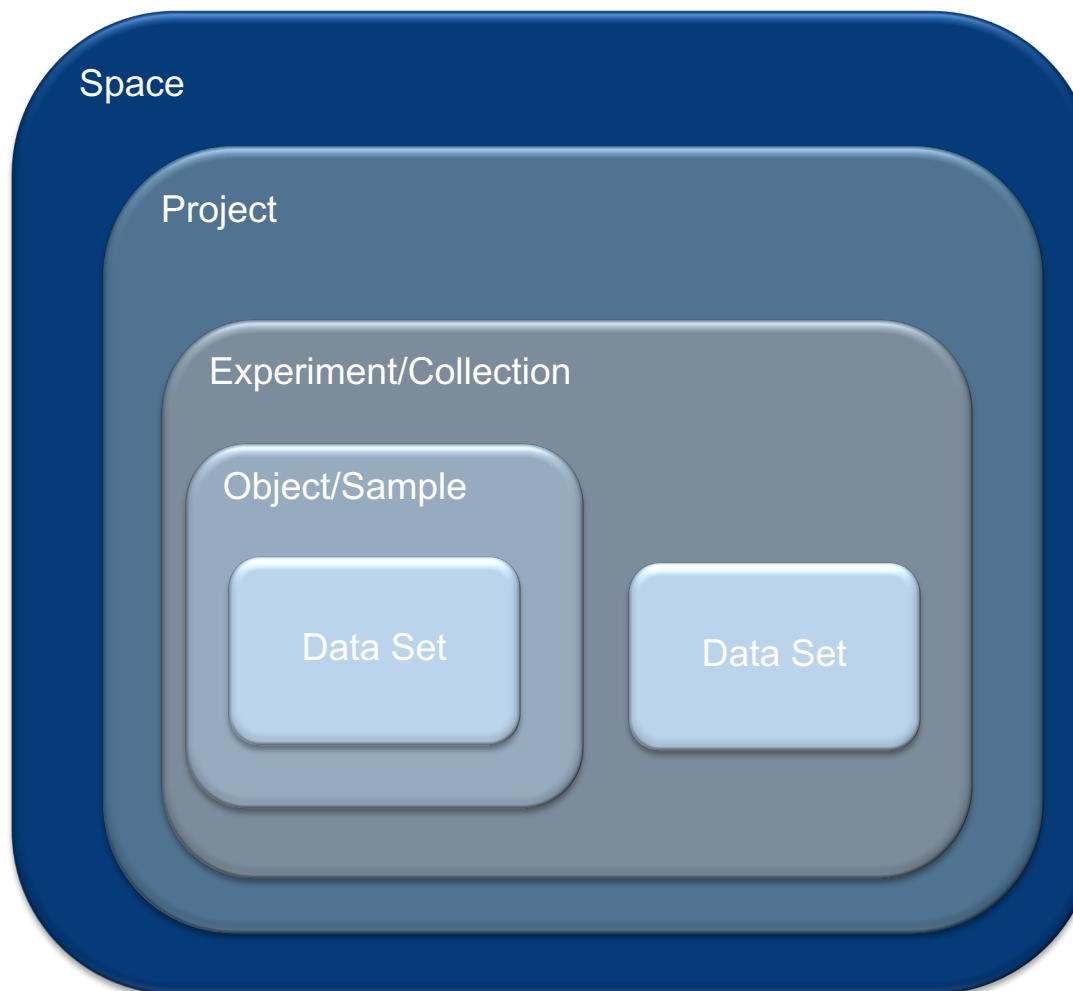
Googledoc to use for questions/communication

<https://docs.google.com/document/d/1uNApJq3jgtYYWGxtwM15ct47LYsE0-UIT92gA6Gcddw/edit?usp=sharing>

Overview of training course

1. Introduction to basic openBIS concepts
2. Hands-on tutorial:
 1. Registration of samples
 2. Registration of protocols
 3. Recording experiments and uploading data
 4. Data analysis with Jupyter notebooks
 5. Data analysis with MATLAB

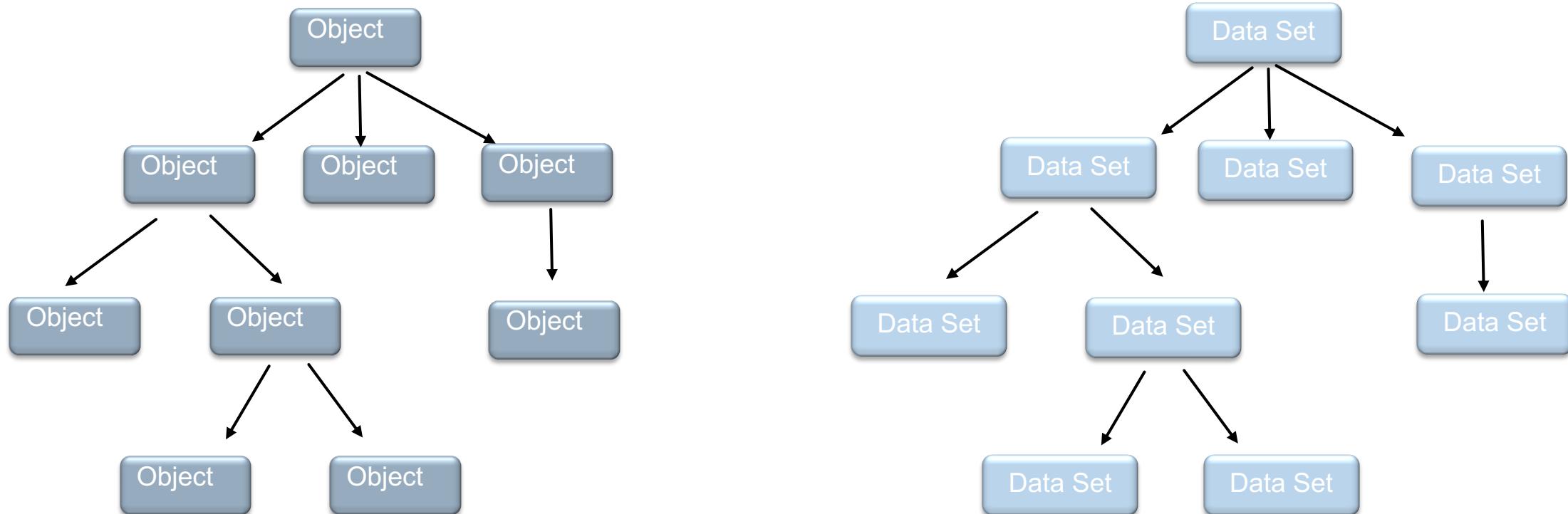
openBIS data structure



- 1. Folder with only code**
- 2. Folder with code + description**
- 3. Folder with code + user-defined properties.**
There can be several types of Experiment/Collection, each defined by different properties. Example: *microscopy experiment, PCR experiment, etc...*
- 4. Basic entity with code + user-defined properties.** There can be several types of Objects/Samples, each defined by different properties. Examples: *Antibody, Chemical, Sensor, Chip, General protocol, Experimental Step...*
- 5. Folder for storing data files with code + user-defined properties.** There can be several types of Data sets, each defined by different properties.

Linking objects and datasets

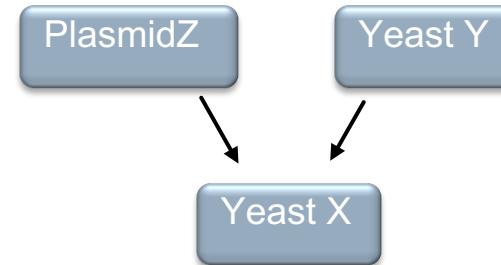
- Objects can be linked to other objects, datasets to other datasets with $N:N$ relationship
- In openBIS terms, these are “parent-child” relationships



What are “parents” and “children”?

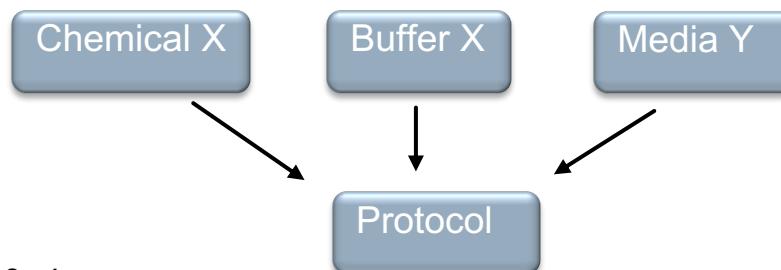
- They are a way of connecting entities together.
- Examples:

1. You make a sample from other samples.



Yeast X is made inserting **Plasmid Z** into **Yeast Y**.
These are assigned as parents to **Yeast X**.

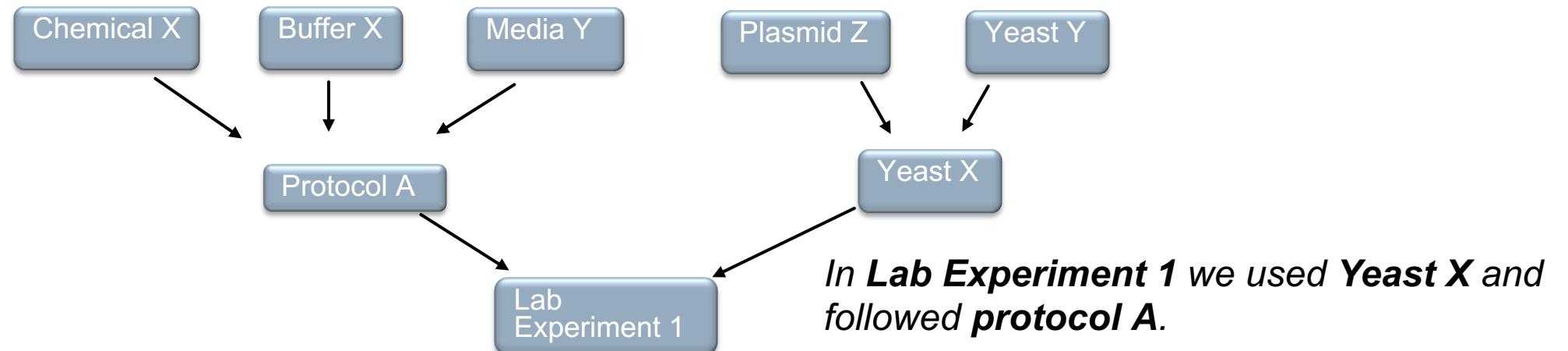
2. You write a protocol, and want to keep track of the samples used.



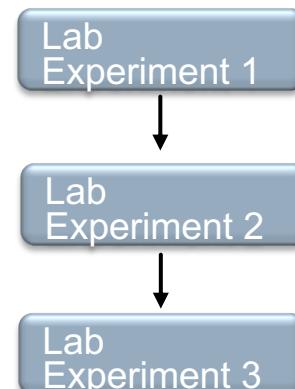
Chemical X, **Buffer X** and **Media Y** are needed to perform the steps described in this protocol. They are parents of this protocol.

What are “parents” and “children”?

3. You describe an experiment and you want to keep track of the protocol(s) and samples used



4. You make one experiment in several steps and you want to link each step to the previous one



Roles

Role	Capabilities
Observer (Space or Instance)	Read-only access to given spaces or to the whole instance.
Space/Project user	Create + edit Object, Experiment. Edit Project .
Space/Project power user	User rights +create Projects . Delete object, experiment, project, datasets. Add, update vocabulary terms.
Space/Project admin	Power user rights+ list roles; create and delete space roles; edit datasets.
Instance admin	Space admin rights + create types. Has access to everything.

Freezing entities

It is possible to “freeze” every level of the openBIS hierarchy.

Space: Default Lab Notebook

+ New Project More ... ▾

- Export Metadata
- Export Metadata & Data
- New Jupyter notebook
- Manage access
- Freeze Entity (Disable further modifications)**

Freezing entities

At every level, everything below is always selected to be frozen. Selection can be modified.

Freeze Entity

Choose the entities to freeze (all by default):

Selected	Type	PermId	Name
<input checked="" type="checkbox"/>	Space	DEFAULT_LAB_NOTEBOOK	DEFAULT_LAB_NOTEBOOK
<input checked="" type="checkbox"/>	Project	20190528221459905-1	DEFAULT_PROJECT
<input checked="" type="checkbox"/>	Project	20190611122038970-49	DEMO_PROJECT
<input checked="" type="checkbox"/>	Experiment/Collection	20190611122056078-50	Demo experiment 1
<input checked="" type="checkbox"/>	Experiment/Collection	20190528221459905-14	Default Experiment
<input checked="" type="checkbox"/>	Object	20190611122145679-52	Step 2
<input checked="" type="checkbox"/>	Object	20190611122213447-53	Step 3
<input checked="" type="checkbox"/>	Object	20190611122127059-51	Step 1
<input checked="" type="checkbox"/>	Object	20190528221828470-42	test
<input checked="" type="checkbox"/>	DataSet	20190611123601400-54	test data

Enter your password to freeze the entities, after they are frozen no more changes will be allowed:
This operation is irreversible!

Password (*):

Accept Cancel



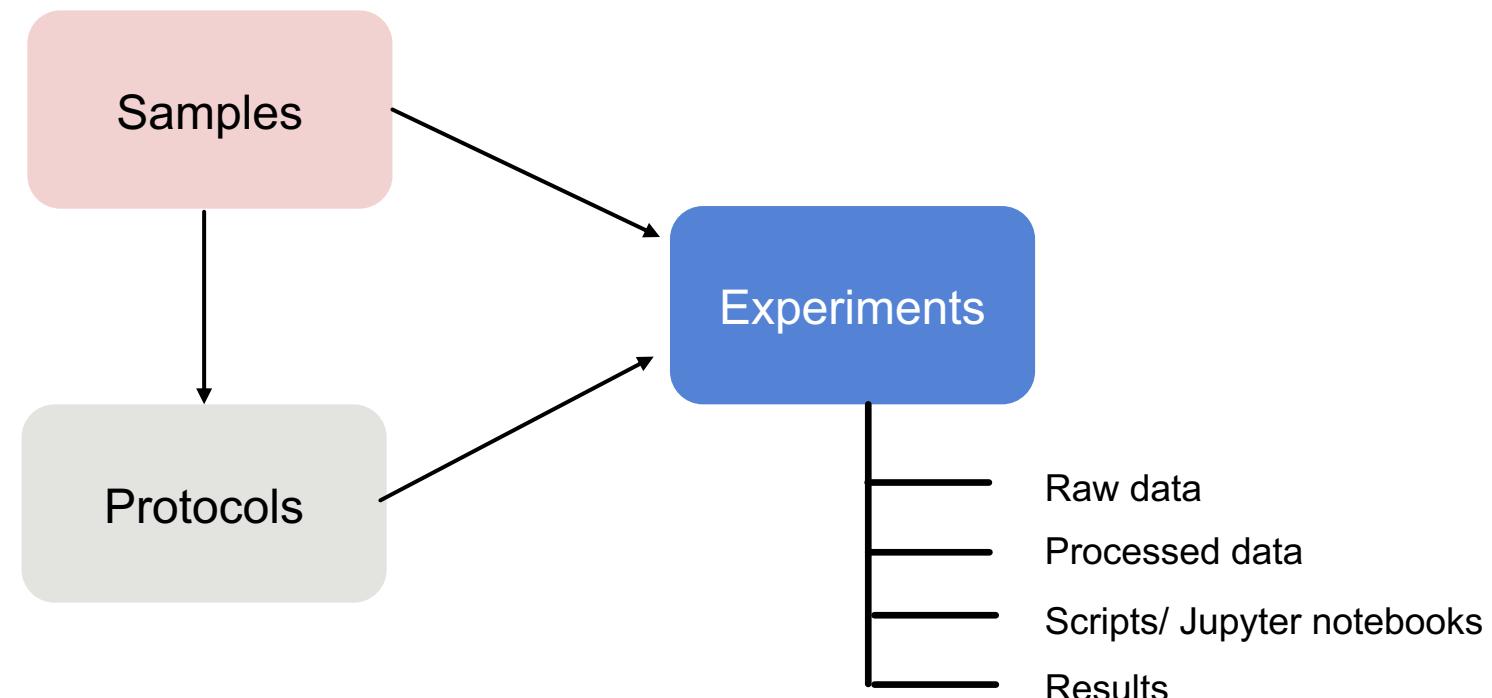
How to use the openBIS Inventory & Lab Notebook

Inventory

Shared by all lab members.

Lab Notebook

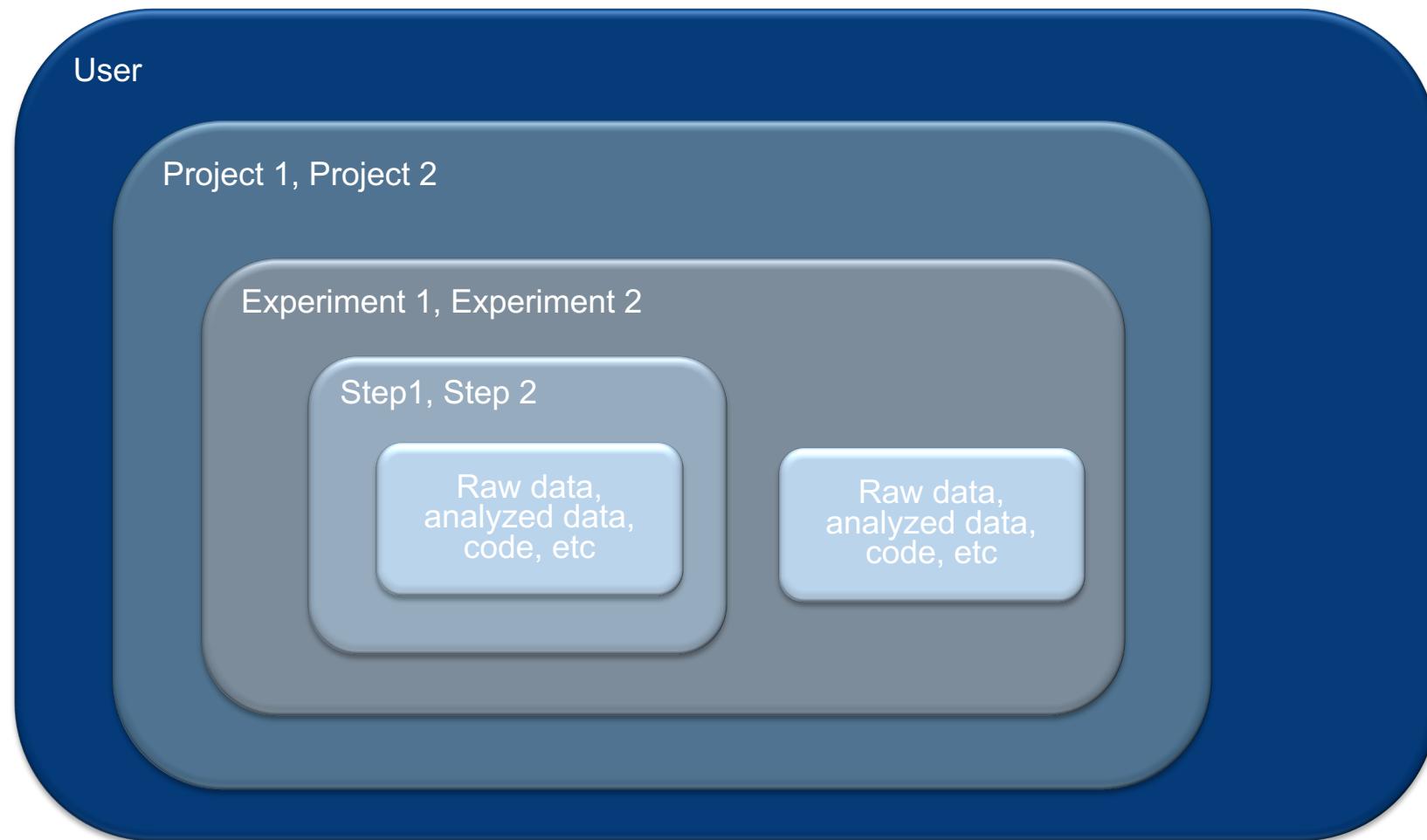
Personal space. Can be shared.



Organization of openBIS Lab Notebook

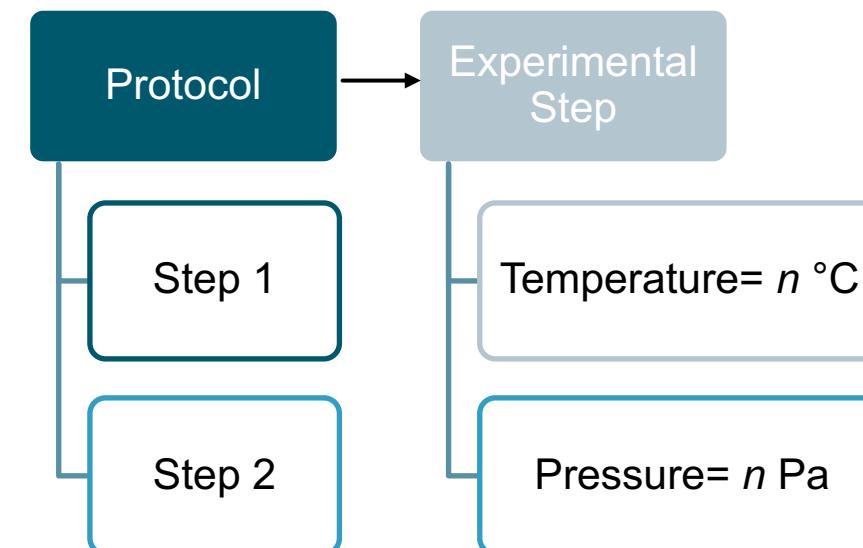
- In the Lab Notebook part of openBIS, usually each user has a **personal Space** where to organize **Projects** and **Experiments**
- An openBIS **Experiment** is a specific scientific question. The single attempts to answer this question can be modelled as **Experimental Steps**.
- **Experimental Steps** can be linked to samples, protocols, other Experimental Steps
- Data (raw, processed, analysed, final results) can be attached to Experiments or Experimental steps in **Datasets**

openBIS Lab notebook



Protocols or Experimental Steps?

- Protocols are standard procedures used in the lab that need to be shared with all lab members
- Every time a given protocol is followed when performing one Experimental Step, the protocol can be linked as parent and the experimental details should be recorded in the Experimental Step itself.



Example

Protocol: muffins recipe

Ingredients

2 medium eggs
125ml vegetable oil
250ml semi-skimmed milk
250g golden caster sugar
400g self-raising flour (or same quantity plain flour and 3 tsp baking powder)
1 tsp salt
100g chocolate chips or dried fruit such as sultanas or dried cherries (optional)

Method

- 1.** Heat oven to 200C/180C fan/gas 6. Line 2 muffin trays with paper muffin cases. In a large bowl beat 2 medium eggs lightly with a handheld electric mixer for 1 min.
- 2.** Add 125ml vegetable oil and 250ml semi-skimmed milk and beat until just combined then add 250g golden caster sugar and whisk until you have a smooth batter.
- 3.** Sift in 400g self-raising flour and 1 tsp salt (or 400g plain flour and 3 tsp baking powder if using) then mix until just smooth. Be careful not to over-mix the batter as this will make the muffins tough.
- 4.** Stir in 100g chocolate chips or dried fruit if using.
- 5.** Fill muffin cases two-thirds full and bake for 20-25 mins, until risen, firm to the touch and a skewer inserted in the middle comes out clean. If the trays will not fit on 1 shelf, swap the shelves around after 15 mins of cooking.
- 6.** Leave the muffins in the tin to cool for a few mins and transfer to a wire rack to cool completely.

Experimental Step: making muffins

- I use 240 ml of whole milk, instead of 250 ml semi-skimmed
- I add a teaspoon of sodium bicarbonate
- I cook the muffins for 30 mins at 180°C

The protocol gives me directions and defines the steps; When I perform my experiment I can change some parameters and this needs to be recorded.



Overview of today's openBIS tutorial

Example: RNA sequencing study of 8 different dog breeds

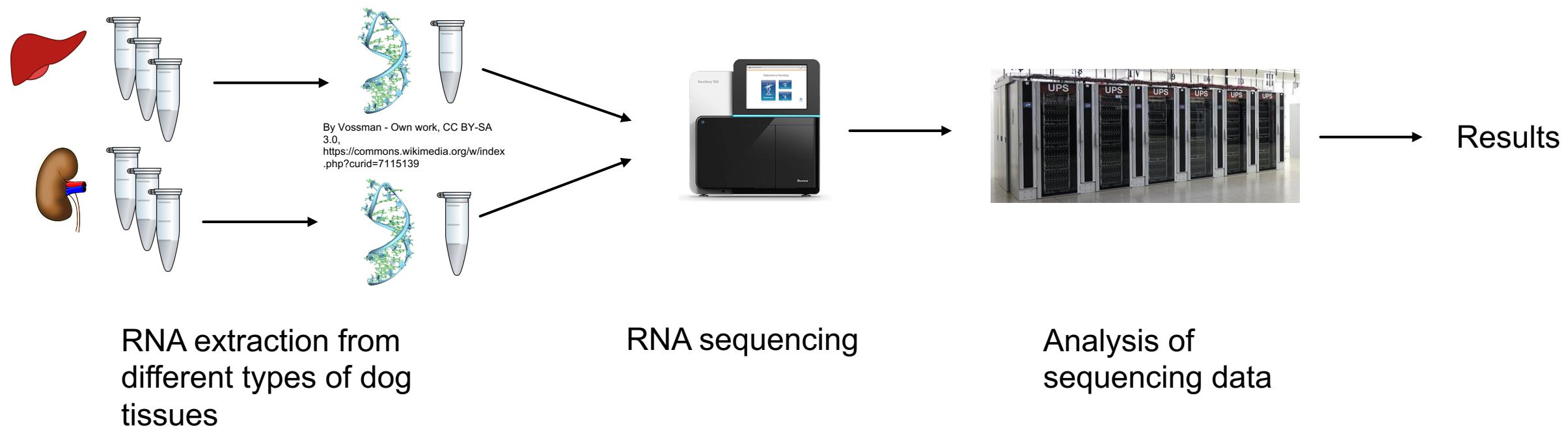
Goal of the study: *understand intra breed genetic variability of dogs with special reference to Beagle dog, since Beagles are used as an animal model for compound testing in the pharma industry.*

The eight different dog breeds are as follows:

1. Beagle
2. GSD
3. Golden Retriever
4. Terrier
5. King Charles
6. Poodle
7. Rottweiler
8. West Highland White Terrier



Overview of the study process



Overview of the study process

Experiments:

1. RNA extraction
2. RNA sequencing
3. Data analysis

Protocols:

1. RNA extraction
2. RNA sequencing

Samples:

1. Tissues
2. Chemicals
3. RNA extracts

How does the process look like in openBIS?

– Inventory

–  Barillac Materials

–  Samples

 Chemicals

 RNA extracts

 Tissues

–  Barillac Methods

–  Protocols

 RNA extraction protocols

– Lab Notebook

–  My Space (Barillac Barillac)

–  Rna Sequencing Of 8 Dog Breeds

–  RNA sequencing

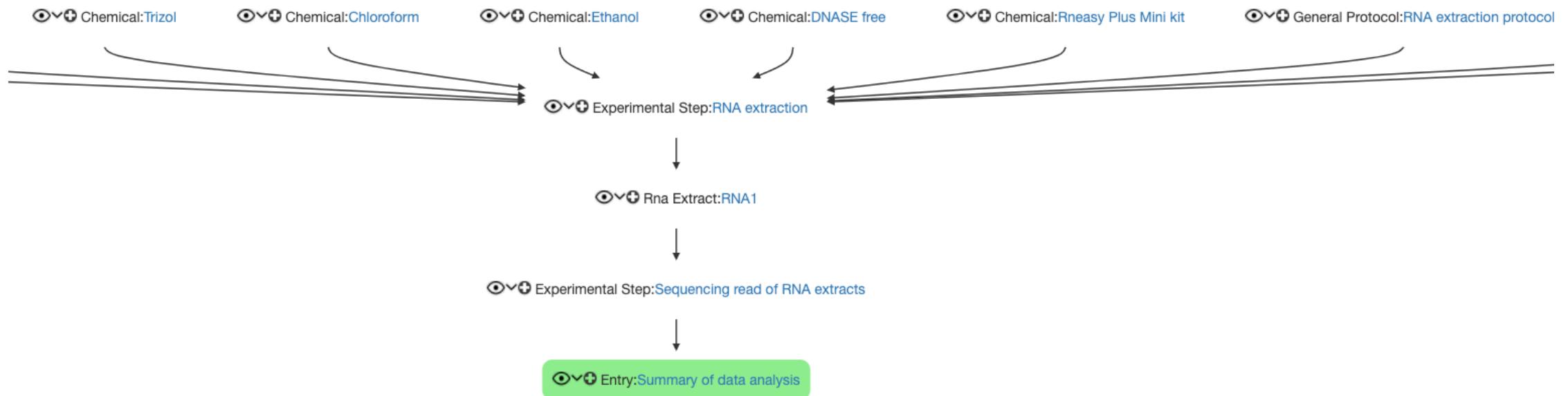
–  RNA extraction

–  Sequencing read of RNA extracts

 RNA seq data

+  Summary of data analysis

How does the process look like in openBIS?

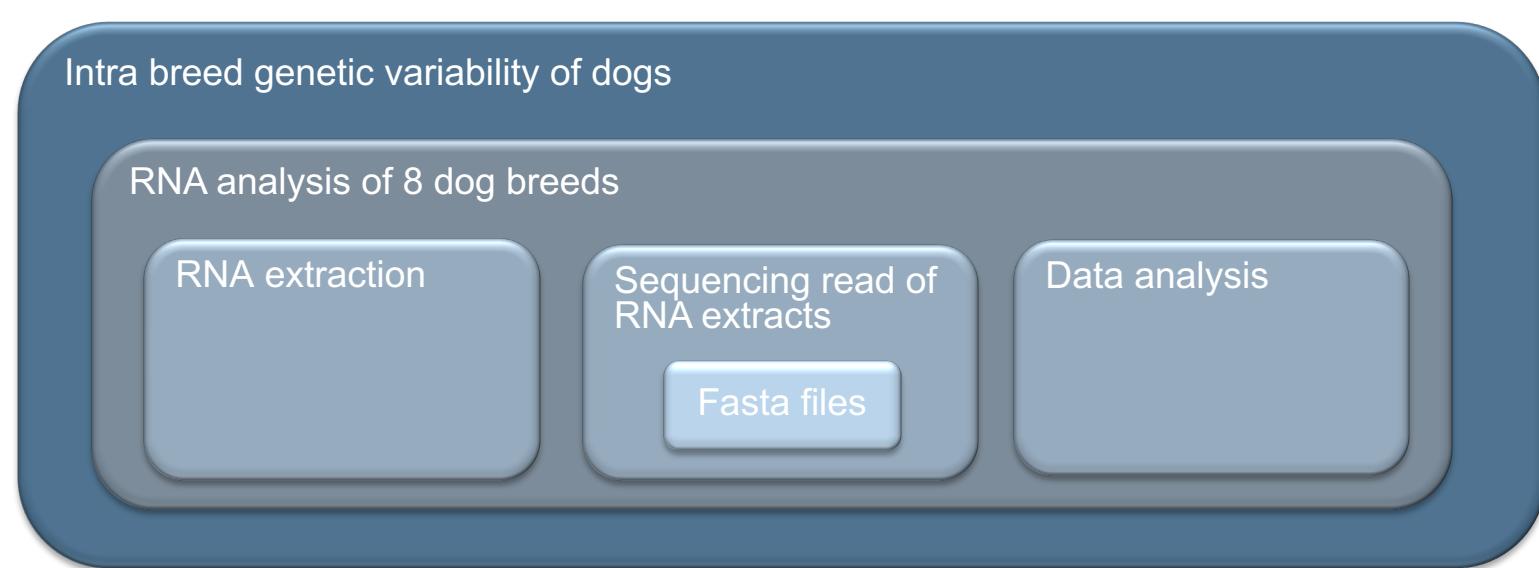


Management of samples and protocols

We will register a few samples and one protocol in the inventory, covering different topics:

1. Single sample registration
2. Batch registration of samples
3. Batch modification of samples
4. How to assign storage positions to samples
5. How to register a standard lab protocol

Lab notebook



- We will create **1 Project, 1 Experiment and 3 Experimental Steps** in your personal space.
- We will see how we can **link** samples and protocols stored in the Inventory to the Experimental Step.
- We will **upload data** to the Experimental Step.

Exercise 1

- Registration and copy of tissue samples: *sections 3.1.1 + 3.1.2 on pages 3, 4*



10 min

Exercise 2

- Batch registration of chemical samples: *section 3.1.3, page 4*



5 min

Exercise 3

- Deletion of duplicate objects: *section 3.1.4, page 4*



5 min

Exercise 4

- Batch modification of chemical samples: *section 3.1.5, page 5*



10 min

Exercise 5

- Visualization of storage positions in the Storage Manager: *section 3.2, pages 5,6*

● To do together

Exercise 6

- Registration of RNA extraction protocol: *section 3.3.1, page 6*



5 min

Short break



10 min

Exercise 7

- Registration of project and experiment: section 4.1, 4.2 pages 7,8



5 min

Exercise 9

- Registration of an Experimental Step: *section 4.3, pages 8, 9*



5 min

Exercise 10

- Registration of RNA extracts in Inventory: *section 4.3.1, page 9*
- Registration of RNA sequencing Experimental Step + data upload: *sections 4.3.2, 4.3.3, pages 9, 10*



10 min

Exercise 11

- Registration of Data Analysis Entry: *section 4.3.4, page 10*



10 min

Exercise 13

- Data visualization + data export: *sections 4.3.5, 4.4, page 11*
- To do together

Exercise 14

- Assign access rights to notebook: *section 4.5, page 11*



5 min

Exercise 15

- Searching the ELN: *sections 5.1, 5.1.1., 5.2, pages 12, 13*



15 min

Exercise 16

- Freezing entities: *section 6, page 13*
- To do together

Data analysis with Jupyter notebooks and MATLAB

Henry Lütcke

Contacts & useful info

Documentation & video tutorials: <https://openbis.ch/>

SIS website: <https://sis.id.ethz.ch/>

Twitter: https://twitter.com/ETH_SIS

SIS helpdesk

sis.helpdesk@ethz.ch

Caterina Barillari

caterina.barillari@id.ethz.ch

Priyasma Bhoumik

priyasma.bhoumik@id.ethz.ch

Henry Lütcke

hluetcke@id.ethz.ch