

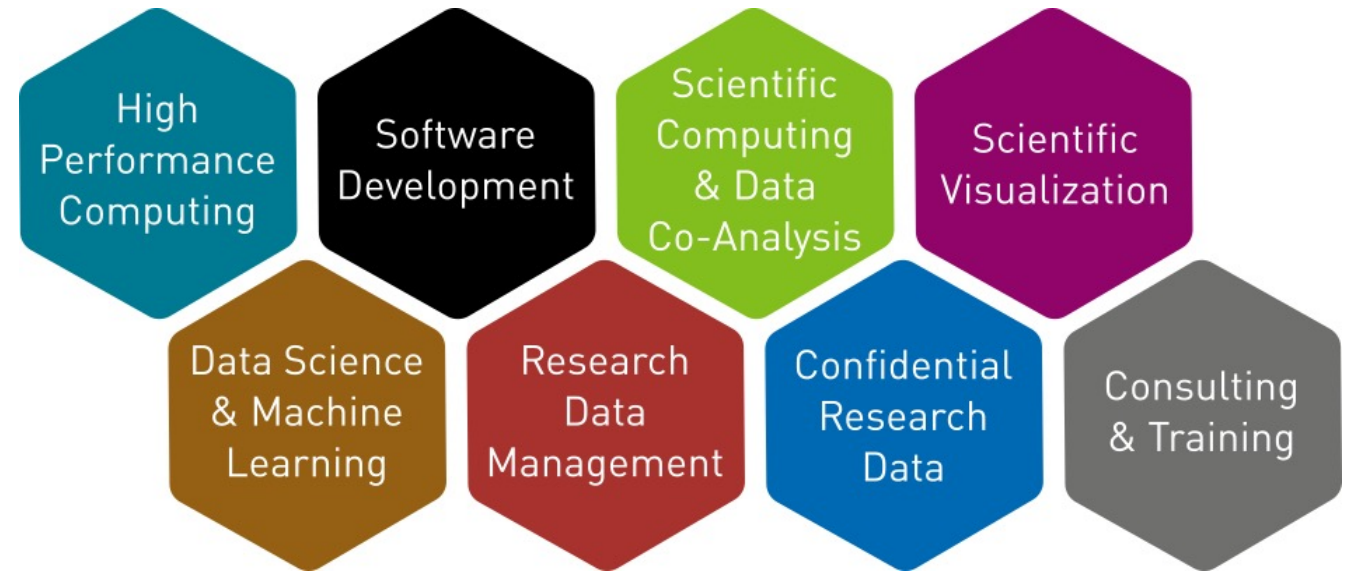
openRDM.swiss: a data management
service for the Swiss academic community

EnhanceR symposium, 2022.11.29

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Scientific IT Services, ETH Zurich



Scientific IT Services of ETHZ



- ❑ A section of ETHZ IT Services
- ❑ >40 experts in various areas of scientific computing
- ❑ With a background in different areas of science

A national RDM service for the academic community

- ❑ Service establishment funded by a swissuniversities P5 project
- ❑ P5 project: 2018-2020
- ❑ Service start: 2021



Cloud-hosted openBIS

- Virtual servers per research group, institute or institution
- Optionally with JupyterHub server for analytics



Self-hosted openBIS

Support for set up on local IT infrastructure



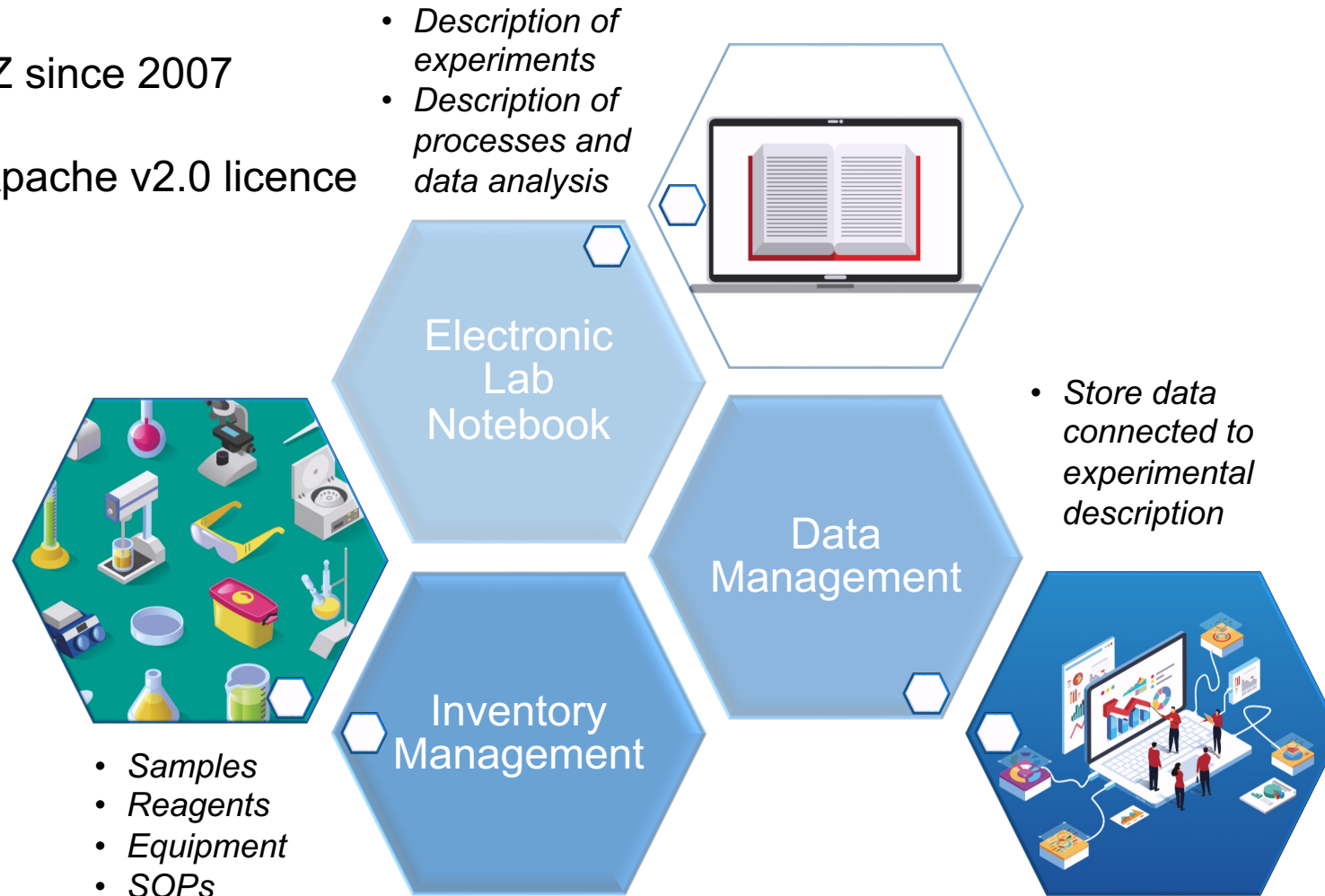
Training & 'best effort' user support



Current customers

openBIS: a complete solution towards FAIR data management

- ❑ Developed at ETHZ since 2007
- ❑ Distributed under Apache v2.0 licence



openBIS Inventory management



Lab equipment

Lab samples & materials

Collection: Mixers

Code	Name	Identifier	Mixing volume	Log Number	Year of registration	Notes	Type	Space	Parents
EQUIPMENT_MIXERS_6	Engh Plus	EQUIPMENTPREPARATION-EQUIPMENT-EQUIPMENT_MIXERS_6	10 L	LOG 139-21.006	2019		Equipment Mixers	EQUIPMENT	
EQUIPMENT_MIXERS_7	Hubert 10	EQUIPMENTPREPARATION-EQUIPMENT-EQUIPMENT_MIXERS_7	8 L	LOG 139-22.901			Equipment Mixers	EQUIPMENT	
EQUIPMENT_MIXERS_1	Telexer inclusion vacuum mixer	EQUIPMENTPREPARATION-EQUIPMENT-EQUIPMENT_MIXERS_1		LOG 139-29.009	2008		Equipment Mixers	EQUIPMENT	
EQUIPMENT_MIXERS_2	Telexer inclusion vacuum mixer	EQUIPMENTPREPARATION-EQUIPMENT-EQUIPMENT_MIXERS_2		LOG 308-29.007	2016		Equipment Mixers	EQUIPMENT	
EQUIPMENT_MIXERS_3	ENVA R 28 M	EQUIPMENTPREPARATION-EQUIPMENT-EQUIPMENT_MIXERS_3	75 L	LOG 139-21.003	1991		Equipment Mixers	EQUIPMENT	EQUIPMENT/EQUIPMENT_MIXERS_3 (Change of st - example)
EQUIPMENT_MIXERS_4	ENVA RV 11	EQUIPMENTPREPARATION-EQUIPMENT-EQUIPMENT_MIXERS_4	390 L	LOG 139-21.004	1999		Equipment Mixers	EQUIPMENT	
EQUIPMENT_MIXERS_5	Engh R 28 M Spix	EQUIPMENTPREPARATION-EQUIPMENT-EQUIPMENT_MIXERS_5	75 L	LOG 139-21.005	2012		Equipment Mixers	EQUIPMENT	

Collection: Chemical admixtures

Code	Name	Identifier	Admixture type	Admixture type other	Date of reception	Manufacturer name	Production date	Mass volumetric density	Solids content	Notes	Type	Space
ADM6	Skagert 705 L	MATERIALSRAW-MATERIALSADM6		OTHER	2021-06-25 14:20:09 +0000	Sika		800.0			Admixture	WATERU
ADM7	W-D STARVIS S 2100 F SAP	MATERIALSRAW-MATERIALSADM7		OTHER	2020-04-20 21:00:00 +0000	SASF					Admixture	WATERU
ADM8	Onix 400	MATERIALSRAW-MATERIALSADM8	Resin		2017-09-27 07:00:00 +0000						Admixture	WATERU
ADM9	Sika Wandfest Superplasticizer	MATERIALSRAW-MATERIALSADM9	Superplasticizer		2019-12-19 15:48:33 +0000	Sika	2020-01-02 15:48:33 +0000	1080.0			Admixture	WATERU
ADM10	Lithium Carbonate	MATERIALSRAW-MATERIALSADM10	Accelerator								Admixture	WATERU
ADM11	No W.A. 130	MATERIALSRAW-MATERIALSADM11	Superplasticizer								Admixture	WATERU

Lab procedures

Samples' storage manager

Box Name: 14
Box Size: 43x
Box Position: A

Barcode reader

User rights management

Collection: Shrinkage

Code	Name	Identifier	Shrinkage dimensionality	Type of time scale (if measured values)	SOP ID	Notes	Type	Space
SHRINKAGE_PROTOCOL_1	SA 3521, Appendix F	METHODSMEASUREMENT_PROTOCOLS-SHRINKAGE_PROTOCOL_1	Linear shrinkage	Unstructured grid (varying time steps) linear scale	4003	Protocol for measuring linear shrinkage of concrete specimens according to the Swiss standard SA 3521 (Appendix F).	Shrinkage Protocol	METHODS

openBIS Electronic Lab Notebook

Experimental Step: Detection of LexA-ER-B42 induction by flow cytometry

Name: Detection of LexA-ER-B42 induction by flow cytometry
 Owner: Diana Ottoz
 Experimental goals: Analyze the induction of LexA-ER-B42 in a concentration series of beta-estradiol using a fluorescence readout

Parents

Name	Identifier	Comments	Organism	Storage conditions	Stock concentration	Sterilization	Publication	Protocol type	Materials	Time requirement
Yeast FRY418	/MATERIALS/YEASTS/FRY418	LexA-ER-B42 + target					Ottoz et al., Nucleic Acids Research, 2014			
1000X Cycloheximide	/MATERIALS/REAGENTS/FRSOB34	diluted 1/1000, treated for 1/2 hour		+4 degrees	1000X	none				

Personal folder



Entities relations

Data ingestion into openBIS

Web UI (low GBs)

Python API (low GBs)

“Dropbox” (high GBs)

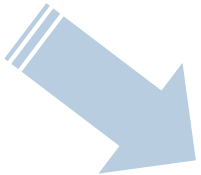
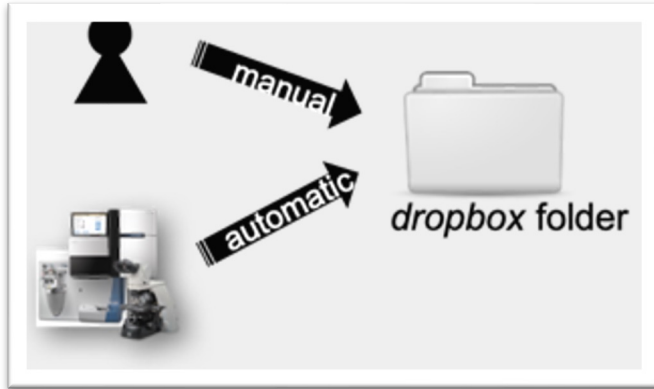
Experimental Step: Detection of LexA-ER-B42 induction by flow cytometry

General

Experimental goals: Analyze the induction of LexA-ER-B42 in a concentration series of beta-estradiol using a fluorescence readout.

Experimental results: The LexA-ER-B42 induction can be measured by using a target gene encoding a fluorescence protein. LexA-ER-B42 induction is different at different concentrations of inducer.

```
ds_new = o.new_dataset(  
    type = 'ANALYZED_DATA',  
    experiment = '/SPACE/PROJECT/EXP1',  
    sample = '/SPACE/SAMP1',  
    files = ['my_analyzed_data.dat'],  
    props = {'name': 'some good name', 'description': '...'}  
)  
ds_new.save()
```



Data

Experimental Step: Detection of LexA-ER-B42 induction by flow cytometry

Experimental goals: Analyze the induction of LexA-ER-B42 in a concentration series of beta-estradiol using a fluorescence readout.

Experimental results: The LexA-ER-B42 induction can be measured by using a target gene encoding a fluorescence protein. LexA-ER-B42 induction is different at different concentrations of inducer.

Identifier	Comments	Details	Suppliers	Type	Modification Date
ANALYZED_DATA/EXP1/SAMP1	LexA-ER-B42 - target			Test	2022-04-20 16:41:28
ANALYZED_DATA/EXP1/SAMP1	about 1:1000, tested for 12 hour	Disable in DMSO, Repeat		Buffer	2022-04-20 17:07:27
ANALYZED_DATA/EXP1/SAMP1	1:2 concentration series with 2000 uM	Disable in		Solution	2022-04-20

Data analysis: openBIS & Jupyter Notebooks

Space: Barillac Barillac

- + New Project
- More ...
 - Export Metadata
 - Export Metadata & Data
 - New Jupyter notebook

```
File Edit View Insert Cell Kernel Widgets Help Not Trusted Python 3 C
```

Datasets Download

```
In [12]: ds0.download(files=ds0.file_list, destination='./', wait_until_finished=True)
Files downloaded to: ./20190328133056219-504
Out[12]: './'
```

Read and display the data

```
In [ ]: img = imread('./20190328133056219-504/original/blobs.tif')
fig = plt.figure(figsize=(10,5))
fig.add_subplot(121)
plt.imshow(img, cmap='gray')
plt.title('blobs')
fig.add_subplot(122)
plt.hist(img.ravel(), bins=10)
plt.title('Histogram of blobs')
plt.show()
```

Saving the results

The next cell stores a copy of this notebook as an html file so it can be open easily in browsers without the need of Jupyter, save before executing this to get the latest version as html

```
In [ ]: from nbconvert import HTMLExporter
import codecs
import nbformat
exporter = HTMLExporter()
output_notebook = nbformat.read(fileName, as_version=4)
output_resources = exporter.from_notebook_node(output_notebook)
codecs.open(fileName + '.html', 'w', encoding='utf-8').write(output)
```

Sets the owner of the result dataset

```
In [ ]: owner = o.get_object('/SIS_HLUETCKE/DEMO/JUPYTER-DEMO'),
owner
```

Creates the result dataset

openBIS + JupyterHub server

Experimental Step: jupyter-demo

- + New
- Edit
- Upload
- More ...

General info

Name: jupyter-demo

Show in project overview: true

Start date: 2020-01-14 11:27:08 +0000

- RAW_DATA : 20200114134628751-71
 - blobs.tif (63.6 kb)
- ANALYZED_DATA : jupyter notebook demc
 - test 5.ipynb (6.6 kb)
 - test 5.ipynb.html (281.8 kb)

JupyterLab-openBIS extension:
<https://pypi.org/project/jupyterlab-openbis/>

Data publication: export to Zenodo



The screenshot shows the 'Zenodo Export Builder' interface. On the left is a navigation menu with categories like Lab Notebook, Inventory, Stock, Utilities, Exports, Storage Manager, User Manager, Trashcan, Settings, Other Tools, and About. The 'Exports' section is expanded, showing 'Export to Zenodo' as the selected option. The main area displays a tree view of the openBIS structure. A blue arrow points from the 'Inducible Transcription Factor' folder to the 'Export Selected' button. Below the tree view, there are instructions: 'You can select any parts of the accessible openBIS structure to export: If you select a tree node and do not expand it, everything below this node will be exported. To export selectively only parts of a tree, open the nodes and select what to export.' and 'Publication time constraint: After the resource has been exported it should be published in Zenodo UI within 2 hours. Otherwise, the publication metadata will not be registered in openBIS.'

On the right, the Zenodo 'New upload' form is visible. It includes a search bar, a 'Save' button, and a 'Publish' button. The form has several sections: 'Files' (showing 'content.zip' with a size of 1.4 MB), 'Communities' (with a search input), 'Upload type' (with options like Publication, Poster, Presentation, Dataset, Image, Video/Audio, Software, Lesson, Physical object, Workflow, Other), and 'Basic information' (with fields for Digital Object Identifier, Publication date, and Title). A blue box with a white dot and the text 'Title' points to the 'Title' field in the 'Basic information' section.

☐ Integration also with ETH data repository

Acknowledgements – openBIS & RDM team



Juan Fuentes



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Rostyslav Kuzyakiv



Henry Lütcke



Swen Vermeul



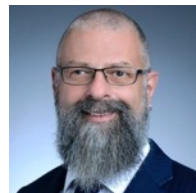
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Artur Pedziwilk



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RP Group Head



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Contacts & useful info

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

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

Mastodon: https://universeodon.com/@ETH_SIS

openBIS support

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