openBIS tutorial

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Caterina Barillari
caterina.barillari@id.ethz.ch

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Overview

In this tutorial we will learn how to use the openBIS inventory and lab notebook.

The tutorial covers the registration of samples, protocols and experiments:

1. Registration of media, chemicals, buffers, plasmid, yeasts
2. Registration of flow cytometry protocol
3. Description of experiments in the lab notebook
4. Data upload
5. Searching the ELN
6. Freezing entities

We will see different ways of registering and updating samples and we will see how to keep track of connections to entities in the system.

Additional documentation and video tutorials can be found at: https://labnotebook.ch/.

Registration of samples and protocols in the Inventory

This part of the tutorial covers the registration of new samples and protocols in the lab inventory.

Registration of new materials and samples in the Inventory

We will start by registering a few samples in the Materials inventory: *media, chemicals, plasmid, yeasts, buffers*. We will see:

1. How to register single samples
2. How to batch register samples
3. How to batch update samples
4. How to assign storage positions
5. How to set relationships with other samples

Registration of a media sample

We will now register one single media sample.

1. Select the **Media Collection** folder in the **Samples** folder
2. Click the **+** button in the main page
3. Enter **Liquid S media** in the **Name** field
4. Enter **To grow cells in well controlled nutritional conditions** in the **For what** field
5. Select **Saccharomyces cerevisiae** in the **Organism** field
6. Select **room temperature** from the **Storage conditions** list
7. **Save**

Click on the **Media Collection** folder. From the **Columns** drop down in the table you can choose which fields to visualize. Select **Name, For what**, **Organism**, **Storage Conditions**; deselect **Identifies**, **Code**, **Type**. This information is stored per user, so the selection only has to be made once.

Batch registration of chemical samples

Now we want to register 4 chemicals. We will do this by Batch Registration.

1. Select the **Chemicals Collection** folder in the **Samples** folder
2. Select **Batch Register Objects** from the **Operations** drop down menu
3. Select **Chemical** from the **Object Type** dropdown menu
4. Download the **template** file and open it with Excel
5. Remove the **identifier** column. This is done to use identifiers automatically generated by openBIS. Keep this column if you want to manually enter identifiers (e.g. /USERNAME_MATERIALS/SAMPLES/CHE1).
6. Fill in the **Name**, **Art. Number** and **Supplier** as below

NAME	SUPPLIER	ARTICLE_NUMBER
Dimethyl sulfoxide (DMSO)	Sigma-Aldrich	D5879
Ethanol (EtOH)	Fluka	02860-2.5L
Beta-estradiol	Sigma	E8875
Cycloheximide	Sigma	C7698

7. Go back to the ELN interface
8. Choose to upload the file you just saved
9. **Accept**
10. Select **Name**, **Art. Number, Supplier** and **Supplier** from the **Columns** drop down in the table.

Batch modification of chemical samples

When we registered the chemicals before, we forgot to enter the information about the storage conditions. To correct this in all samples, we can batch update the samples:

1. Select the **Chemicals Collection** folder in the **Samples** folder
2. Select only **Identifier, Name** and **Storage Conditions** from the **Columns** dropdown
3. Select **Export visible columns with visible rows** from the **Options** dropdown list
4. Edit this file with Excel:
    a. enter **RT** under the Storage column in the first 3 rows
    b. Enter **4** under the Storage column in the last row
    c. **Save** the file
5. Go back to the ELN
6. Select **Batch Update Objects** from the **Operations** list
7. Select **Chemical** from **the Object Type** list
8. Select the previously modified file from the Documents
9. **Accept**

The storage info has now been added to the chemicals.
Storage is *a Controlled Vocabulary* in openBIS, i.e. a list of pre-defined values to choose from. The list of available *Controlled Vocabularies* is available under **Utilities -> Vocabulary Browser.** By clicking on one Vocabulary, the list of terms can be visualized. When using batch upload/update, the **Code** of the Vocabulary term needs to be entered in the template file.

Registration of a plasmid sample with storage info

1. Go to the **Plasmid Collection** folder in the main menu
2. Click the + button
3. Enter **insul-(lexA-box)4-PminCYC1-CitrineA206K-TCYC1** in the **Name** field
4. Select **pRS30y** from the **Backbone** list
5. Select **bla** from **the Bacterial antibiotic resistance** list
6. Select **URA 3** from the **Marker** list

7. Enter NotI, KpnI in **the Flanking Restriction Enzymes** field
8. Enter a storage position:
    a. Click the + button under the storage table
    b. Select the **-80°C Room A1.2** freezer
    c. Select the **1,1** rack
    d. Enter **Username_Plasmid_box** in the **Box Name** field
    e. Select the **10 x 10** size
    f. Select position **A1**
    g. Accept
9. **Save**

Registration of yeast samples with parents

First we will register one yeast:

1. Go to the **Yeasts Collection** folder in the main menu
2. Enter **LexA-DBD-long-HBD-B42** in the **Name** field
3. Select **BY4741** from the **Genetic Background** list
4. Select **a** from the **Mating Type** list
5. Select **met15-** from the **Background-specific markers** list
6. Select **ura3- leu2-** from the **Common markers** list
7. Select **cir+** from the **Endogenous 2micron plasmid in yeast** list
8. Select **transformation** from the **Origin** list
9. Select **PCR** from the **Strain Check** list
10. Enter a storage position:
    a. Click the + button under the storage table
    b. Select the **-80°C Room A1.2** freezer
    c. Select the **2,1** rack
    d. Enter **Username_Yeast_box** in the **Box Name** field
    e. Select the **10 x 10** size
    f. Select position **A1**
    g. Accept
11. **Save**

Now we will register a second yeast, which was made using the first yeast and the previously registered plasmid. These can be set as **parents.**

We can **copy** the yeast we just register and modify only certain fields that are different:

1. Go to the **Yeasts Collection** folder in the main menu
2. Click on the **existing yeast** sample
3. Click on the **copy** button from the **menu toolbar**
4. Leave everything unselected
5. **Accept**
6. The new yeast is created. Edit the form.
7. Remove **LexA-DBD-long-HBD-B42** from the **Name** field and enter **demo.**
8. Add relationships:
    a. Add yeast parent:
        i. In the parents section, click on the **+** next to **Yeast parents**

ii. Select **the yeast previously registered** from the table

b. Add plasmid parent:

i. Click the **+** next to **Plasmid**

ii. Select the only plasmid in the table

iii. Select **integration** from the **Plasmid Relationship** dropdown

iv. Enter **URA3** in the **Plasmid annotation** field

9. Change value to **leu2-** for the **Common markers** field
10. Enter a storage position:
    a. Click the **+** button under the storage table
    b. Select the **-80C Room A1.2** freezer
    c. Select the **Username_Yeast_box** in the **2,1** rack
    d. Select position **A2**
11. **Accept**
12. **Save**
13. Visualize the connections to the plasmid and yeast with the hierarchy tree button 

Visualization of storage positions with the Storage Manager

The openBIS storage manager offers an overview of all storages configured for the lab:

1. Select **Storage Manager** under **Utilities**
2. Select the **-80°C room A1.2** storage from the **Storage** list
3. Click on one of the boxes and visualize the content

It is possible to drag & drop boxes to change the position of a box inside a storage (or to a different storage). In the same way the position of a sample inside a box can be changed (this is not supported for multiple positions for the same sample).

Batch registration of buffer samples with parents

We will now register 3 buffers using batch registration**.** Each of the buffers has 2 chemicals as parents, which we need to set in the file.
The first buffer, cycloheximide, has DMSO and cycloheximide as chemical parents. The second and third buffers, bet-estradiol, have Ethanol and beta-estradiol as chemical parents.

Setting parents in file:

1. Open the **buffers.tsv** file with Excel to visualize its content
2. Go to the **Chemicals Collection**
3. Select **Identifier** and **Name** from the table
4. In the **buffers.tsv** file, fill in the **parents** column with the **Identifiers** corresponding to the chemicals mentioned above:
    i. DMSO and cycloheximide for the first buffer
    ii. EtOH and beta-estradiol for the second and third buffer

Batch upload

5. Go to the **Buffers Collection** folder in **Samples** in the main menu
6. Select **Batch Register Objects** from the **Operations** drop down menu
7. Select **Solution Buffer** from the **Object Type** list
8. Select the **buffers.tsv** file just modified
9. **Accept**

Select **Name, Parents, Details, For what, Stock Concentration and Storage Conditions** from the **Columns** dropdown.

Click on one of the entities in the table (e.g. cycloheximide) and visualize the connections to the chemicals with the hierarchy tree button 

Deletion of duplicate Objects

In the step above we registered 3 buffers, but two of them are the same. We want to delete one of them:

1. Go to the **Solutions Buffers Collection** folder in **Samples** in the main menu
2. Select *Object* **beta-estradiol** from the table (select button in first column)
3. Select **Delete selected** from the **Options** drop down in the table
4. Enter **duplicate** in the **Reason** field
5. **Accept**

When *Objects* (and also *Experiments/Collections*) are deleted they are first moved to the trashcan, In order to be completely removed from the database they have to be deleted also from the trashcan. Alternatively, it is also possible to revert deletion from the trashcan, if something was accidentally moved here.

1. Go to the **Trashcan** under **Utilities** in the main menu
2. Select **Delete Permanently** from the **Operations** drop down in the table
3. Read the warning message
4. **Accept**

Registration of a new protocol in the Inventory

We will now register a flow cytometry protocol in the Methods Inventory.

Registration of a flow cytometry protocol

1. Open the **flow-cytometry-protocol.docx** file from the training material
2. Go to the ELN
3. Go to the **Flow cytometry protocols** folder in the main menu
4. Click on the **+** button in the main page
5. Copy/paste the corresponding fields from the doc file in the ELN form
6. To add the chemical as parent:
    a. Click the + button next to **Links to Materials and Methods**
    b. Select **Chemical** from the drop down
    c. Select **Name** from the **Columns** drop down
7. Select **cycloheximide** from the table
8. **Save**

Laboratory Notebook

In the laboratory notebook, usually each lab member has a personal folder (=*Space*) to organize *Projects* and *Experiments*. *Experiments* can be further divided in *Experimental Steps*. An openBIS *Experiment* is a specific scientific question and it contains *Experimental Steps* that are individual attempts to answer it.

Experimental Steps can be linked to each other (if needed) and they can also be linked to materials and methods stored in the Inventory.

Some examples:

Lab Experiment	**Corresponding openBIS data model**
Monitor decondensation upon transcriptional activation of a given insert in some strains. This experiment involves 3 different steps: 1. Make some plasmids 2. Make reporter strains for decondensation using plasmids made before–> PCR results 3. Test strains made before in different conditions -> raw data, MATLAB code	**Experiment**: Monitor decondensation upon transcriptional activation of a given insert in some strains. **Exp Step 1**: make plasmids **Exp Step 2**: make reporter strains for decondensation using plasmids made in Exp step 1 (*can be a child of Exp Step 1*) **Exp Step 3**: test strains made in Exp Step 2 using condition 1 (*can be a child of Exp Step 2*) **Exp Step 4**: test strains made in Exp Step 2 using condition 2 (*can be a child of Exp Step 2*) **Exp Step 5**: test strains made in Exp Step 2 using condition 3 (*can be a child of Exp Step 2*) Each *Experimental Step* can contain the data related to it.
Induction of a transcription factor in standard growth conditions with synthetic complete medium containing 2% of glucose. This experiment involves 3 different steps: 1. Detection of transcription factor induction by flow cytometry 2. Detection of transcription factor induction by Western blotting 3. Detection of transcription factor induction by Western blotting	**Experiment**: Induction of a transcription factor in standard growth conditions with synthetic complete medium containing 2% of glucose. **Exp Step 1**: flow cytometry **Exp step 2**: western blotting 1 **Exp Step 2**: western blotting 2 In this case we are trying different methods to detect the transcription factor, but there is no connection between them. Each *Experimental Step* can contain the data related to it.
Monitor the expression of a given gene. This experiment involves 2 steps: 1. RT-qPCR 2. Western blotting	**Experiment**: Monitor the expression of a given gene **Exp Step 1**: RT-qPCR **Exp Step 2**: Western blotting Each *Experimental Step* can contain the data related to it.

As an example, we work on a project where we study different inducible transcription factors. In this project we perform several experiments. For example, in one experiment we analyze the abundance of 4 variants of a transcription factor before and after induction. The analysis is done by western blotting.
In another experiment we induce the transcription factor in standard growth conditions and we detect it by flow cytometry and 2 types of western blotting.
In openBIS we would need to register:

1. 1 *Project*
2. 2 *Experiments*
3. 1 *Experimental Step* for the first experiment; 3 *Experimental Steps* for the second experiment.

In this tutorial we will work with **Example 2** described above and we will register 1 *Project*, 1 *Experiment* and 1 flow cytometry *Experimental Step*. In the Experimental Step, we will create links to samples and protocols stored in the inventory.

Registration of a Project

We want to register a project called **Inducible transcription factor**:

1. Select your folder in the Lab Notebook part of the main menu
2. Click the **+** button in the main page
1. Enter **Construction and characterization of a beta-estradiol-inducible transcription factor for Saccharomyces cerevisiae** in the **Description** field
2. Enter **Inducible_transcription_factor** in the **Code** field
3. **Save**

Please note that Projects only have **Codes**, not names. The Code can only have alphanumeric characters and no spaces. It is recommendable to use "_" to separate words. The ELN will translate this to a space in the main menu.

Registration of an Experiment

In the Project registered before, we want to register a first Experiment, called **Induction of a transcription factor in standard growth conditions with synthetic complete medium containing 2% of glucose:**

1. Select the Project folder
2. Click the **+** button in the main page
3. Enter **Induction of a transcription factor in standard growth conditions with synthetic complete medium containing 2% of glucose** in the **Name** field
4. Check **Show in project overview.** This is a way to mark important experiment, so that they are shown in the Project page. Usually this would be done at the end of the Experiment.
5. Enter **12.11.2019** in the **start date**
6. Enter **02.12.2019** in the **end date**
7. Enter **Analyze the transcription factor in a concentration series of inducers** in the **Experimental goals** field
8. Enter **Both variants of transcription factor tested induced in a concentration series of inducer. The variant LexA-ER-B112 is stronger than LexA-ER-B42.** in the **Experimental results** field.
9. **Save**

Registration of a first Experimental Step

Now we want to register an *Experimental Step*, which is a flow cytometry experiment. We also want to create links to samples and protocols stored in the inventory.

1. Click the **+** button in the Experiment page
2. Enter **Detection of LexA-ER-B42 induction by flow cytometry** in the **Name** field
3. Click **Show in project overview**

Now we want to create links to materials and methods stored in the Inventory. We want to add a link to *1 media, 2 buffers, 1 yeast* and *1 protocol*. These are the samples and materials we used in this experimental step and the protocol we followed.

4. Add media:
    a. Click the **+** button next to **Parents**
    b. Select **Media** from the list
    c. Show the Media **Name** in the table (Columns dropdown)
    d. Select the only media available in the table
5. Add buffers:
    a. Click the **+** button next to **Parents**
    b. Select **Solutions Buffer** from the list
    c. Show the **Names** of the buffers in the table (Columns dropdown)
    d. Check both buffers in the table
    e. Select **Add selected** from the **Options** dropdown in the table
6. Add yeast:
    a. Click the **+** button next to **Parents**
    b. Select **Yeast** from the list
    c. Show the **Names** of the yeasts in the table (Columns dropdown)
    d. Select the **demo** yeast
7. Add protocol:

    When we add a protocol we have two options:

        i. Create a link to an existing protocol in the inventory. This is suitable when the protocol is followed "as it is"
        ii. Copy the protocol to our experiment folder in the lab notebook in order to modify it. This is suitable when the main protocol is modified during the experiment.

    We will now see the procedure to create a local copy:
    b. Click + next to **General Protocols**
    c. Show the **Name** of the protocols in the table (Columns dropdown)
    d. Select the flow cytometry protocol
    e. Choose **Use as template** from the **Operation** dropdown in the table
    f. Enter **a code** in the **Code** field
    g. Accept
    h. Right click on the Protocol code and open in new tab. This is a copy of the original protocol, created in your personal folder (check the identifier). You can see that this protocol is linked to the original protocol in the inventory. In this way you can modify your local copy and leave

the template untouched. If you do not need to make any modification to the protocol, you do not need to use the **Use as template** option.

8. **Save**

Visualize the connections to the samples and protocols with the hierarchy tree button  .

Data upload to an Experimental Step

Data can be uploaded to *Experiments* or *Experimental Steps* using the same procedure.

In the same way, files can also be added to *Objects* in the Inventory (i.e. to samples or protocols).

In this case we want to upload: 1. the raw data that was obtained from the flow cytometer; 2. the R script that was used to analyze the data.

Upload raw data

1. Click the **Upload Dataset** icon  from the **menu toolbar**
2. Select **Raw data** from the **Data Set type** dropdown
3. Enter **Flow cytometry data** in the **Name** field
4. Select the **FC_LEXA-ER-B42-raw.zip** file in the **Documents** folder to upload
5. Check **Uncompress before import**
6. **Save**
7. Open the **Raw data** folder in the Experimental step to see the content

Upload the R script

1. Click the **Upload dataset** icon  from the **menu toolbar**
2. Select **Source Code** from the **Data Set type** dropdown
3. Type **flow** in the **Parent** field and select the dataset that comes up in the list. This step is not necessary, but it allows you to establish a relationship between datasets. In this case we establish a connection to the raw data that was analyzed with the R script we are uploading.
4. Enter **R script** in the **Name** field
5. Select the **FC_LEXA-ER-B42-script.R** file in the **Documents** folder to upload
6. **Save**
7. Open the **Code** folder in the Experimental step to see the content

Image upload in Experimental Step Results

We now want to upload an image in the **Results** section of the *Experimental Step*:

1. **Edit** the Experimental Step
2. Scroll down to the **Experimental Results** section
3. Click the image icon  in the text editor
4. Go to the **Upload** tab
5. Choose the **FRY418t24hCitrine.png** file in the git repository

6. Click **Send it to server**
7. Resize the **width** to 400
8. Press **OK**
9. **Save**

Data visualization

To open data files stored in openBIS we recommend to use software that allows to mount openBIS as a drive on your computer. Examples are:

1. Mountain Duck for MacOS (https://mountainduck.io)
2. NetDrive for Windows (https://www.nsoftware.com/sftp/netdrive/).

Files can be opened with the desired application in read-only mode.

Any other FTP solution can also be used (e.g. Cyberduck, Filezilla, etc).

Please note that **data files stored in openBIS are read-only**!

Data and metadata exports

It is possible to export a complete lab notebook or only parts of it (*Project*, *Experiment*, *Experimental Step*, *Datasets*).

In each folder, the menu toolbar on the main form has an option to **Export metadata only** or **Export metadata+data**. We recommend to export data only if it does not exceed a few GBs.

When you export something, you will receive an email with a link to download your metadata (+data).

The export contains folders with the same structure organization they have in openBIS. Metadata is exported to 4 different file formats: .docx, .html, .txt, .json.

Access rights assignment to a personal notebook or to a specific Project

It is possible to grant collaborators and colleagues access rights to your complete lab notebook or only to selected *Project*(s).

To grant rights to your folder:

1. Select your folder in the Lab Notebook part of the main menu
2. Click the **Manage access** icon  in the main page
3. Select a role from the **Role** dropdown menu. Available roles:
    a. **Observer**: has read-only access
    b. **User**: can create and modify entities, but cannot delete anything
    c. **Admin**: can create, modify and delete entities
4. Select **User** from the **grant to:** dropdown
5. Enter **the username of a registered user**
6. **Grant access**

Searching the ELN

openBIS offers 3 options for searching:

1. **Text search** on all fields stored in the database. Searches can be refined using the **Advanced search**.
2. **BLAST** search for sequence comparison across sequences stored in the database.
3. **Data Set Files** search. This should be used to find files uploaded as datasets by their name.

Generic text search

We want to find all the flow cytometry *Experimental Steps* registered by you.

1. Enter **flow cytometry** in the **Global search** field, on top of the main menu. This search returns a few results. Now we want to narrow down the search.
2. Select **Object** in the **Search For** dropdown
3. Click the + button in the **Criteria** table
4. Select **Property** from the **Field Type** dropdown
5. Select **Object Type** from the **Field Name** dropdown
6. Enter ***STEP*** in the **Field Value** field
7. Click again the + button in the **Criteria** table
8. Select **Property** from the **Field Type** dropdown
9. Select **Registrator** from the **Field Name** dropdown
10. Enter **your username** in the **Field Value** field
11. Run the search

In this case, the search returns only one item, but in a similar way, you can run complex searches by combining multiple search criteria.

Saving and re-using searches

To save a search in your Project folder:

1. Select **Save** on top of the page
2. Enter **demo search** in the **Name** field
3. Enter **Queries** in **the search entity to store query** field
4. **Save**

Run a saved search:

1. Refresh the page to clear the search
2. Select the search from the list of saved searches
3. Run the search

Data Set Files search

We want to find a file that contains “script” in the name.

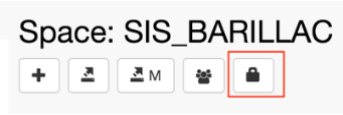
1. Enter **script** in the **Global search** field, on top on the main menu
2. Select **Data Set File** from the dropdown next to it

The search returns the dataset that contains the R file script we uploaded to out flow cytometry experiment before.

Freezing entities

Since the last upgrade (openBIS v19.06.1), openBIS has a new feature that allows to freeze entities that should no longer be modified. When freezing one entity, everything connected to it can be frozen too. The user needs to select what should be frozen and what shouldn't.

Please note that freezing is **IRREVERSIBLE**!



At all levels of the notebook and inventory, there is a **lock** icon.

When you click the lock, you are presented with a list of things connected to the chosen level that can also be frozen. By default, everything is selected. After the selection, you need to enter your password to be able to freeze entities.