Biomaterial Atlas: how to add a biomaterials screen

This document will guide you through the Jupyter Notebook template which is used to create a Biomaterials screen entry for the Biomaterial Atlas. The template can be divided into three section: project level details, study design and study results.

Note: it is assumed you have a basic understanding of Jupyter Notebooks but no programming experience is needed. The Jupyter notebook is available via https://github.com/BioMaterialAtlas/JupyterNotebooks

Project level details

The project level fields will create a key value pair describing the most essential information at a project level.

Study type:

The study type is already defined and you only have to run the Jupyter cell. It is important not to change the study_type key as this is used by the Biomaterial Atlas to load and filter different studies.

```
Provide the study type

In [3]: Study_type = 'Biomaterials Screen'

        You selected the study type: Biomaterials Screen
```

Study ID:

The study ID is a code used to quickly find a study, and consist of the abbreviation of the lab and a 3 digit code (001 being the first study). In the case of the BioInterface Science group, the study ID can also be found in the internal screen database.

```
In [10]: ID = input('Provide the study ID: ')

         Provide the study ID: BIS012
```

Study Name

The study name describes the project in only a few keywords. It is not similar to the study title, which is often the title of the publication.

```
In [4]: Study_Name=input('Provide  the study name (3 keywords): ')

        Provide  the study name (2 keywords): Encapsulation screen
```

For example, when we take the encapsulation screen with the study title: “Foreign body giant cell formation in vitro and the foreign body response in vivo follow distinct topographical design rules.” The title is often not used to discuss a dataset with other researchers but in most cases you use some key words to describe the dataset. In this case we could pick “Encapsulation screen” as the study name.

Project Name

The project name provides the project to which this dataset belongs. A project name is not the same as the study name, since multiple studies can be part of the same project.

```
In [5]: Project=input("Provide the project name: ")
        Provide the project name: Encapsulation Study
```

For example, we can carry out three different screens to study the effect of encapsulation. All three screens will be member of the project: “Encapsulation study” .

Title

The key title can take any value, it can be the title of the publication (recommended) or the title of the unpublished manuscript.

```
In [6]: Title=input("Provide the title of the study (publication title if applicabl
        Provide the title of the study (publication title if applicable): Foreign
        body giant cell formation in vitro and the foreign body response in vivo
        follow distinct topographical design rules.
```

Lead author

The lead author is the first author on the publication, or the lead scientist when no publication is associated with the dataset.

```
Lead_author=input("Provide  the first and last name of the lead author: ")
```

Principal investigator

The principal investigator is often the last author on the paper, or the group leader when the dataset is not associated with a publication.

```
Principal_investigator=input("Provide  the first and last name of the PI: "
```

DOI

The DOI, or Digital Object Identifier, is the identifier associated with the publication. When the dataset is not associated with any publication, you can type “N/A”

```
DOI=input("Provide  the DOI: (if not applicable type N/A): ")
```

Date

The date should be given in the format: DD-MM-YYYY. Where the month is formatted as January/February/../May and so on.

```
Date=input("Provide the date of the study: ")
```

Summary

The summary gives the overall findings and conclusion of the paper. This can be seen as a short abstract of the study

```
Summary=input("Provide  the summary of the study: ")
```

Note: the fields describing the project level details have to be filled in. You cannot skip one questions but are allowed to type “N/A” if you cannot answer it. When you do skip a questions, the Jupyter Notebook will raise an error while saving the file.

Metadata: study design level

The study design metadata describe information about the experimental setup of your dataset. They do not describe the results (hence the metadata study results section) but provide a detailed description of each experiment. The metadata study design section describes many experiments (collected by reviewing multiple projects) and not all experiments have to be carried out in one project. That is why every entry starts with a Yes or No question. When you answer the question with “No”, you can skip all the related questions.

Cell Culture

The first question will ask you if you performed a cell culture:

```
cell_culture_performed = input("Did you perform a cell culture? (Yes or No)
```

```
Did you perform a cell culture? (Yes or No) Yes
```

When you answer this question with “Yes”, you will have to fill in all questions about the Cell Culture. When you answer “No”, you can skip the cell culture questions and go to the next experiment.

Cell type

Provide information on the cell type by answering:

```
Cell_type = input("Provide  the cell type: ")
```

The cell type can be for example: Monocyte, B cell, T cell, hMSC, Glial cell, Fibroblast, and so on.

Passage number

This question will ask you to provide the passage number of your cell:

```
Passage_number = input("Provide  the passage number: ")
```

Cell Medium

The medium section is divided into two categories: start ampule and cell culture. For both categories you are asked to provide the following information:

- Medium type
- Medium Name
- Serum details
- Type of antibiotics used
- Medium component(s)
- Concentration of the component(s)

To explain how to answer those questions, let's take the following example:

HMSCs (donor 8F3543, Lonza) were cultured in basic medium consisting of αMEM (Gibco) supplemented with 10% fetal bovine serum (Lonza) , 2 mM l-glutamine (Gibco), 0.2 mM ascorbic acid (Sigma Aldrich) and 100 U ml^{-1} penicillin +100 g ml^{-1} streptomycin (Gibco).

The medium type is a basic medium for hMSC, thus the answer to the question:

```
start_ampule_type = input("Provide  the type of the start ampule: ")
```

is: hMSC basic medium

The medium name is alpha-MEM, which we can give as an input to:

```
start_ampule_medium = input("Provide  the medium name: ")
```

The medium is supplemented with 10% Fetal Bovine Serum. So we can answer the following question:

```
start_ampule_serum = input("Provide the serum details")
```

with "10% Fetal bovine serum".

Next, we can fill in "Penicillin, Streptomycin" for:

```
start_ampule_antibiotics=input('Provide  the type of antibiotics used: (type none if not used) ')
```

For the medium components, we can fill in "L-glutamine, ascorbic acid" for:

```
start_ampule_components = input("Provide the medium components: ")
```

And "2 mM, 0.2 mM" as values for the medium components concentration:

```
start_ampule_components_concentration = input("Provide  the concentration of the components: ")
```

Please note that the components and components concentration fields should be in the same order. Here, we do not take into account the antibiotics concentration.

Biomaterials screen

The first question will ask you whether you performed a biomaterials screen:

```
biomaterials_screen_performed = input("Did you perform a screen? (Yes or No) ")
```

A biomaterials screen is not limited to a TopoChip but can also be a NanoTopoChip, WellPlate, ChemoTopoChip, Phenom28, or Galapagos Chip. Therefore you are asked to provide the screening type:

```
biomaterials_screen_type = input("Provide the screening type: ")
```

The next question relate to the design of the chip:

```
biomaterials_design_type = input("Provide the design type: ")
```

```
biomaterials_feature_scale = input("Provide the scale of the platform: ")
```

```
biomaterials_base_material = input("Provide the base material information: ")
```

```
biomaterials_surface_treatment = input("Provide the details on surface treatment (N/A if not applicable
```

```
biomaterials_coating = input("Provide details on the material coating: ")
```

The feature scale can be set as micrometer, nanometer, or any other SI metric for scale. If your chip did not have any surface treatment or coating, you can fill in “N/A”.

After providing the number of replicates, you only have to provide a summary of the screen. This summary described what you did and why but leaves out the results (remember this is metadata on a study design level and not study result).

```
biomaterials_summary = input("Provide a summary of the experiment: ")
```

```
Provide a summary of the experiment: Provide a summary of the experiment: The TopoChip platform was u
sed to analyse the responses of monocytes from 3 healthy donors to 2,176 different algorithm-designed
surface topographies. Experiments were performed with a total of 16 TopoChips with each unique topogr
aphy in duplicate, so all topographies were tested 32 times. The monocytes responded strongly to the
physical cues provided by the topographical features evidenced by rearrangement of their F-actin stru
ctures. Quantitative information was acquired by high content imaging and image analysis and the topo
graphies were ranked based on total cell number and average number of nuclei per cell.
```

Fluorescence imaging metadata

This section will ask you to provide the metadata for the fluorescence imaging experiment. Besides the type of microscope and the data of the experiment, it will ask you the following information about the labels:

- First antibody
- Second antibody
- Target
- Fluorescent dye
- Excitation wavelength
- Emission wavelength

The template assumes you have used three different labels (consistent with most existing screens). When you have only used two labels, you have to fill in “N/A” for all the questions related to the 3rd label.

Surface validation

This sections will ask you to provide the metadata for the surface validation experiment. In most cases, a TopoChip screen results in a number of surfaces selected for a more in-depth investigation.

First you are asked to provide the number of selected surfaces for validation. Second, you are asked to provide the surface feature id that has been selected. Third and finally, you are asked to provide the surface id (if they do not match the feature id).

This happened for example in older studies, for example the ALP study by Hulshof et al. There they have given surface ids a different name, so they have to be matched against the feature id from the TopoChip. Please make sure that you match the surface id and the feature id in the right order.

qPCR experiment

This section will ask you to provide the most basic details of a qPCR experiment. To fill in all the fields, you will need information about:

- Experiment type
- Cell type
- Time point(s)
- Read out(s)

Histology experiment

This section will ask you to provide basic details of a histology experiment. You will need to file in the name of the slide scanner and the performed staining. Later on, you will have the opportunity to describe in details the histology results.

Flow cytometry

To add information about a flow cytometry experiment, you will need to provide the following information:

- Cell seeding density
- Culture time
- Medium
- Staining
- Name of the flow cytometry machine
- Number of replicates

When you have applied not one but two or more stains, you can just add them in normal text format:

```
: flow_machine = input("Provide the name of the flow cytometry machine: ")
```

```
Provide the name of the flow cytometry machine: N/A
```

Biomechanical test

To add information about a biomechanical test, you will need to provide the following information:

- Type of biomechanical test (biaxial stress test, compression test, etc)

- Load cell (with unit, so not 2.8 but 2.8 N)
- Applied force (with unit)

Animal study

To add information about an animal test, you will need to provide the following information:

- Organism
- Species
- Sex
- Number of replicates
- Replicates per surface

Metabolic test

To add information about a metabolic test, you will need to provide the following information:

- Type of metabolic test
- Cell type
- Culture time
- Culture medium type

Metadata: study result level

Up till now, you did not add any results to the JSON object, whereas this is the most interesting part of a study. In the next section, we are going to add a summary of the results per experiment.

Biomaterials screen

Here, you can provide a description of the main findings. Here, the idea is not to describe which surfaces are selected (you have already given the feature ids aboven) but whether the cells responded to the topographical features, if certain cell structure show rearrangement, and if the results are observed over the replicates.

Surface validation

Now, it is time to provide a description of the surface validation results. For example, you can write down whether the surfaces selected for a low attachment in a TopoChip screen also have low attachment in the surface validation experiment.

```
surface_validation_description = input("Provide a description of the findings: "
```

```
Provide a description of the findings: Low attachment and fusion topographies s
elected in the TopoChip screen indeed also showed relatively low levels of atta
chment and fusion on the corresponding 15 mm disks. The observed levels of atta
chment were equal to or even lower than on the n-PCU flat surface, and fusion w
as similarly low, with more than 95% of the fusion cells having only 2 and maxi
mally 3 nuclei. In contrast, the high attachment topographies and increased lev
els of fusion in the TopoChip screen, indeed showed the same behavior on the 15
mm disks.
```

qPCR results

When the study contains ax qPCR experiment, you can now provide the main findings of this experiment. When the study does not contain an qPCR experiment, you can skip this part (please make sure that when you skip this part, you should not evaluate the Jupyter cell)

Histology results

When the study contains a histology experiment, you can now provide the main findings of this experiment. When the study does not contain histology experiment, you can skip this part (please make sure that when you skip this part, you should not evaluate the Jupyter cell).

You can be as descriptive as possible, since more information might be useful in the future.

```
histology_results_description = input("Provide a description of the main finding
```

```
Provide a description of the main finding: Fueled by the large differences in t
he number of adherent macrophages and the induction of FBGCs, we expected a cor
relation between adherence in vitro and the degree of FBR in vivo. However, to
our surprise, we did not find that correlation. We did see marked differences i
n FBR parameters in our quantitative histological data, in line with literature
where topography and pore size influence the degree of encapsulation. Many para
meters were measured in our analysis, but the most relevant ones are the fibros
is score, capsular thickness and collagen content, as these correlate with impl
ant failure. Surface 1584, a high adhesion surface, showed the thinnest capsule
with the fewest number of FBGCs. Surface 731 at the other end of the spectrum s
howed low adhesion in vitro and precisely had the highest scores for FBR parame
ters. The areas described above suggest an inverse correlation, but this is not
confirmed by the 3 other areas that lie between these two extremes. Therefore,
we conclude that we do not see a relationship between macrophage attachment and
FBGC formation in vitro and encapsulation in vivo.
```

Flow cytometry results

When the study contains a flow cytometry experiment, you can now provide the main findings of this experiment. When the study does not contain a flow cytometry, you can skip this part (please make sure that when you skip this part, you should not evaluate the Jupyter cell).

Biomechanical test results

When the study contains a biomechanical test experiment, you can now provide the main findings of this experiment. When the study does not contain a biomechanical test, you can

skip this part (please make sure that when you skip this part, you should not evaluate the Jupyter cell).

Metabolic activity results

When the study contains a metabolic activity experiment, you can now provide the main findings of this experiment. When the study does not contain a metabolic activity, you can skip this part (please make sure that when you skip this part, you should not evaluate the Jupyter cell).

Create a JSON object

Once you have answered all the questions, it is time to create a JSON object to store the data. This is quite straightforward and you only have to change the file name.

First, we create the study_design_items object:

```
study_design_items=[]
```

You can evaluate the Jupyter cells and if you did not skip any Yes/No questions you should be able to evaluate all cells successfully.

```
if cell_culture_performed.upper() =='YES':
    cell_culture_object={
        'Name':'Cell culture',
        'Cell_type':Cell_type,
        'Passage_number':Passage_number,
        'Medium':{
            'Start_ampule':{
                'Type':start_ampule_type,
                'Medium':start_ampule_medium,
                'Serum':start_ampule_serum,
                'Antibiotics':start_ampule_antibiotics,
                'Medium_components':start_ampule_components,
                'Medium_components_concentration':start_ampule_components_concen
            },
            'Seeding_medium':{
                'Type':seeding_medium_type,
                'Medium':seeding_medium_medium,
                'Serum':seeding_medium_serum,
                'Antibiotics':seeding_medium_antibiotics,
                'Medium_components':seeding_medium_components,
                'Medium_components_concentration':seeding_medium_components_conc
            }
        }

    }
    study_design_items.append(cell_culture_object.copy())

if biomaterials_screen_performed.upper() =='YES':
    biomaterials_screen_object={
        'Name':'Biomaterials screen',
        'Type':biomaterials_screen_type,
        'Design':biomaterials_design_type,
        'Feature_scale':biomaterials_feature_scale,
        'Base_material':biomaterials_base_material,
        'Surface_treatment':biomaterials_surface_treatment,
        'Coating':biomaterials_coating,
        'Number_of_replicates':biomaterials_number_of_replicates,
        'Summary':biomaterials_summary
    }
```

For the study results, you just have to evaluate the Jupyter cells to create the study_results_items.

```
study_results_items=[]
```

```
if biomaterials_screen_performed.upper() =='YES':
    screen_results_object={
        'Name':'Biomaterials screen results',
        'Description':screening_description
    }
    study_results_items.append(screen_results_object)
if surface_validation_performed.upper() =="YES":
    surface_results_object={
        'Name':'Surface validation results',
        'Description':surface_validation_description
    }
    study_results_items.append(surface_results_object)
```

Now we can add all the information to the JSON object:

```
document={
    'Study_type':Study_type,
    'ID':ID,
    'Name':Study_Name,
    'Project':Project,
    'Title':Title,
    'Lead_author':Lead_author,
    'Principal_investigator':Principal_investigator,
    'DOI':DOI,
    'Date':Date,
    'Summary':Summary,
    'Study_design':study_design_items,
    'Study_results':study_results_items
}
```

If you know how to read a JSON object structure, you can print the document and see if the structure looks like you expect.

```
{'Study_type': 'Biomaterials Screen',
 'ID': 'BIS012',
 'Name': 'Encapsulation screen',
 'Project': 'Encapsulation Study',
 'Title': 'Foreign body giant cell formation in vitro and the foreign body re
sponse in vivo  follow distinct topographical design rules.',
 'Lead_author': 'Chantal M. Diedrich',
 'Principal_investigator': 'Jan de Boer',
 'DOI': 'N/A',
 'Date': 'Jan 2014',
 'Summary': 'We recently employed our TopoChip screening platform to define d
esign principles for macrophage binding and maturation in vitro, and in this
manuscript we extend this to foreign body response in vivo. We first assessed
foreign body giant cell (FBGC) formation in vitro on 2,176 different topograp
hies  and learned that small pillars and sufficient space in between them res
```

Write the JSON object to an JSON object

Now we are ready to save the JSON object to our hard drive. You only need to change the file name:

write to json file

Please give a new to save the json object

```
file_name="Encapsulation_BMA.json"
```

```
import json
```

```
with open(file_name, 'w') as outfile:
    json.dump(document, outfile)
```