CEPLAS
Cluster of Excellence on Plant Sciences

Organizing Weberlab experimental data

December 9th, 2020

Dominik Brilhaus

CEPLAS data science and management

Academic experts in data science

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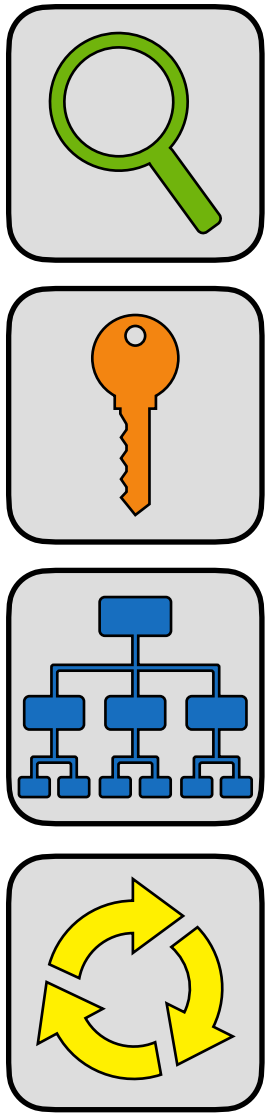
Data management officer

Björn Usadel

- Head of Bioinformatics Institute (IGB-4) @ Jülich
- Head of Institute for Biological Data Science @ HHU

FAIR principles of data stewardship



Findable

Accessible

Interoperable

Reusable

Wilkinson, M., *et al.* (2016)
The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data* **3,** 160018.
https://doi.org/10.1038/sdata.2016.18

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Community-integrated plant research data

CEPLAS institutes

CEPLAS

hhu

JÜLICH

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Data Science and Management

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DataPLANT
Community

DataPLANT

nfdi4plants.de

Local computing infrastructure

RRZK
fdm.uni-koeln.de
ZIM
fdm.hhu.de

F A I R

CEPLAS
Research data
platform

Public repositories

*Findable, Accessible, Interoperable, Reusable

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And the winners are…

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Data Management Representatives of the Weber Lab

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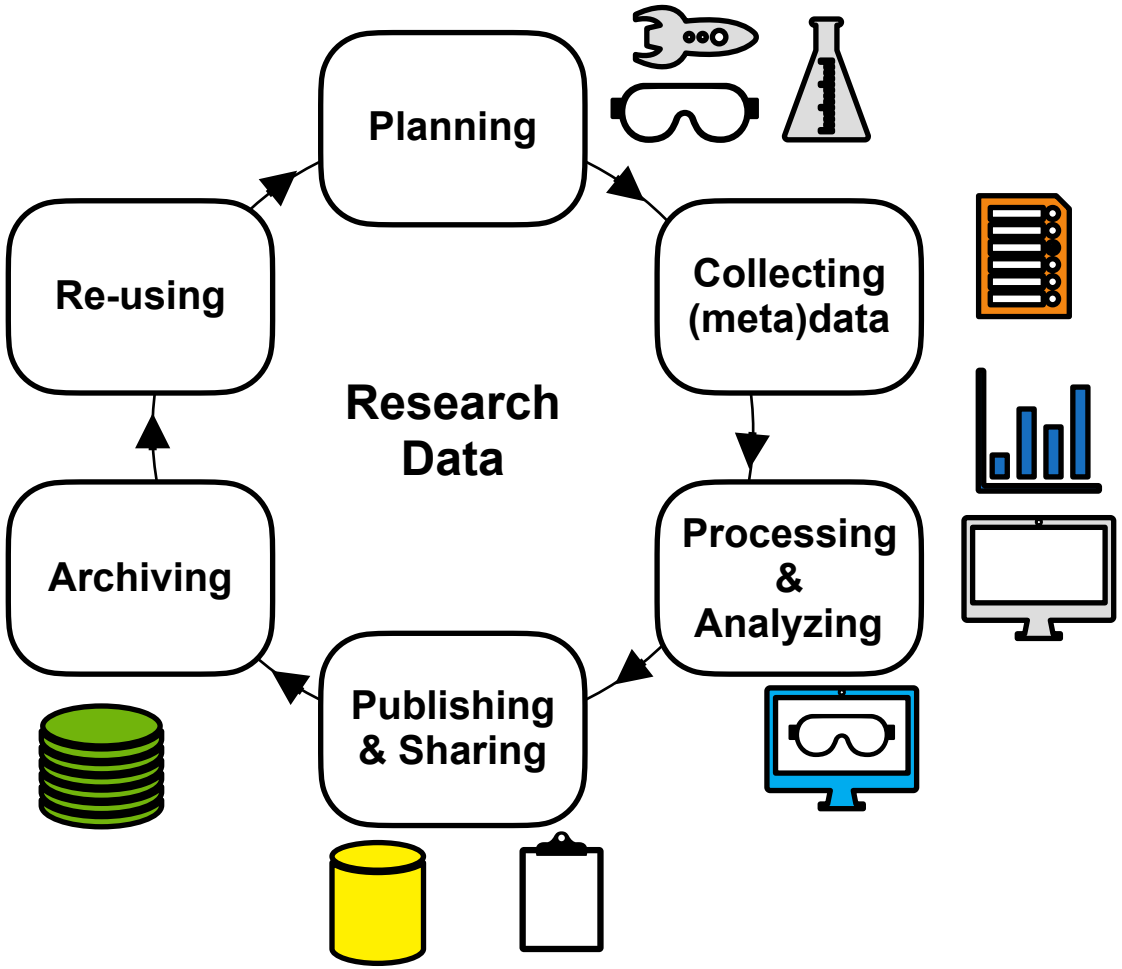
The research data cycle



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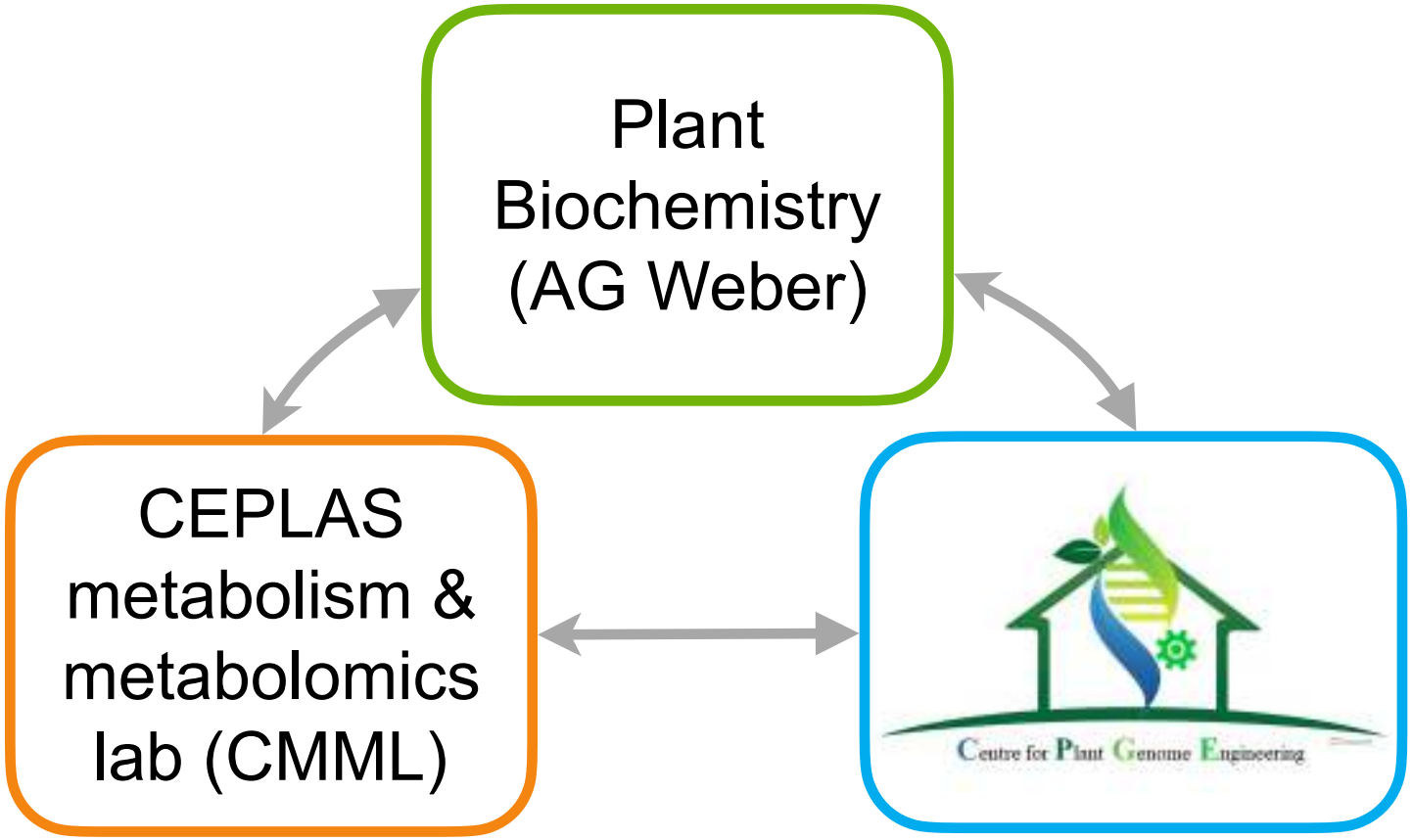
Goals

- Quick intro to the electronic lab notebook “elabFTW”
- Introduce a lab catalog to share resources between



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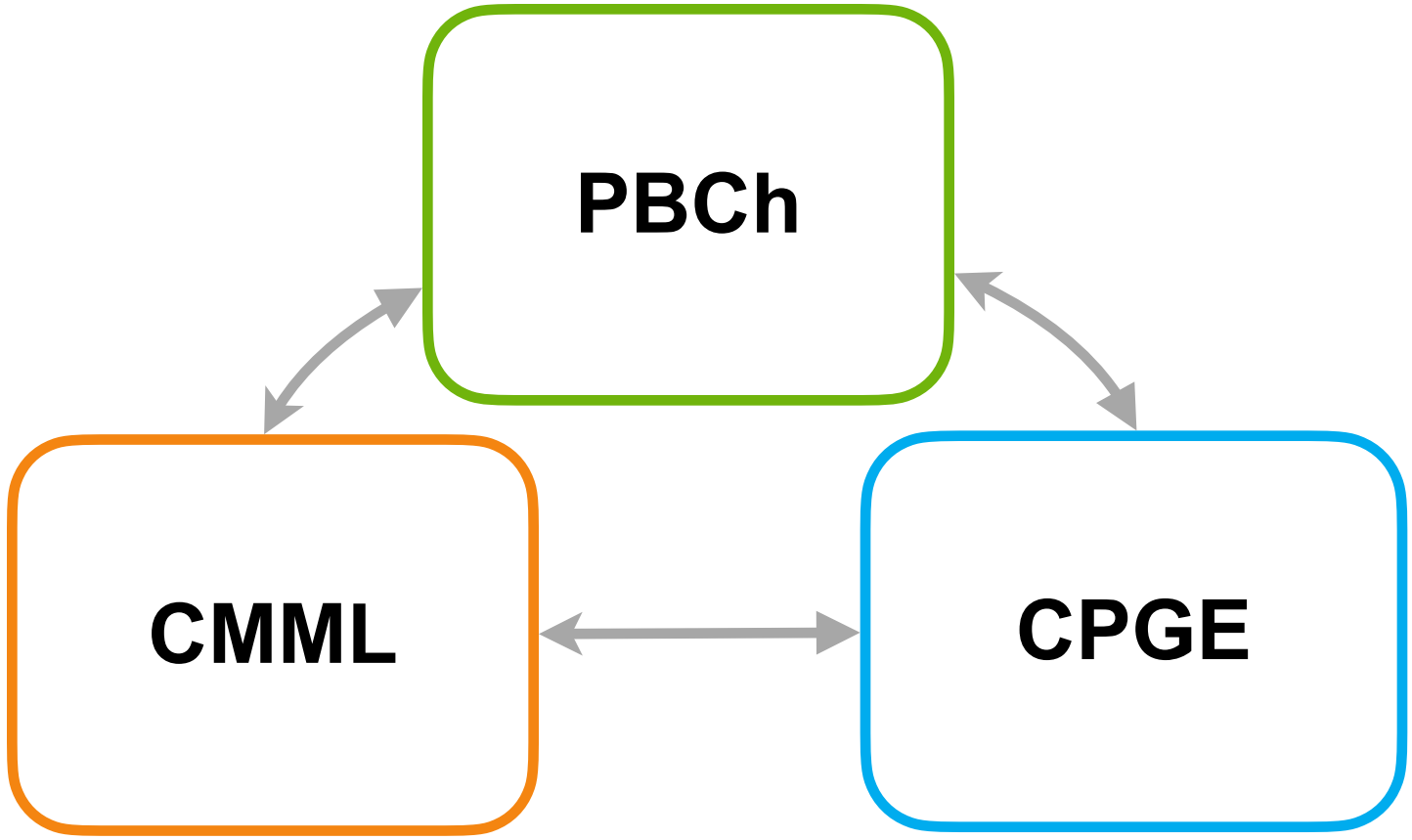

Why using an ELN

- Document anything “from green house to digital data object”
  - Biological materials
  - Lab methods
  - Lab instruments
  - Sample processing
- Catalog and share lab resources
- Boost reproducibility
- Boost traceability

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elabFTW - Getting started

- Register at: https://elabftw.hhu.de/register.php
  - Team “Plant Biochemistry”
  - Use your @hhu.de email address

- Login at https://elabftw.hhu.de/login.php

ELN resources @ HHU

- ELN softwares: elabFTW, Labfolder
  - https://www.fdm.hhu.de/fdm-tools/elektronische-laborbuecher.html
- Tutorials
  - https://mediathek.hhu.de/playlist/410
- NRW ELN Wiki
  - https://wiki.hhu.de/display/ELB
- Rocketchat channel
  - https://rocketchat.hhu.de/channel/elb_eln

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Intro to elabFTW

Creating an experiment

- Edit mode
  - Tags
  - Date
  - Status
  - Title
  - Experiment
  - Steps
  - Linked items
  - Attachments, etc.
  - The three dots

- View mode
  - Duplicate
  - PDF
  - ZIP
  - Lock
  - Share
  - Time-stamp
  - Commenting

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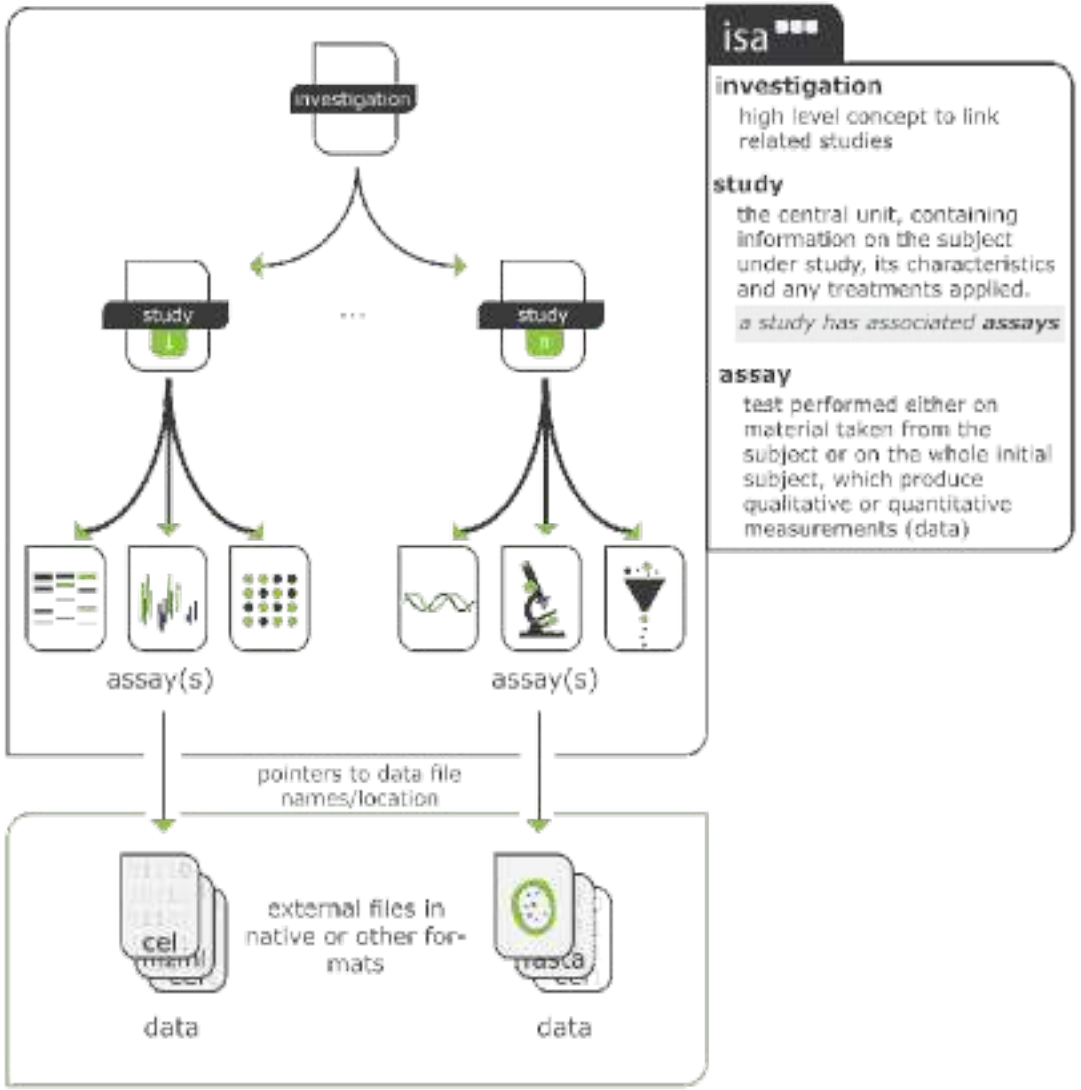
The ISA Model of (experimental) metadata

- **Investigation**
  - Overall goals
  - Scientific context
- **Study**
  - Experimental steps
- **Assay**
  - Leading to (raw) data

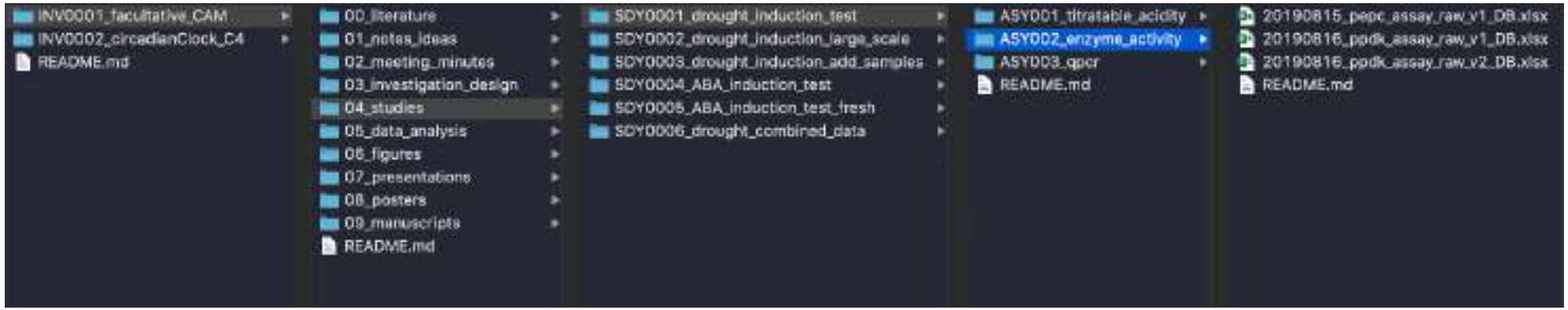


https://isa-tools.org/format/specification.html

Directory structure

Any system is better than none → document your system

- Establish a system (e.g. in your lab) and use it consistently
- Example
  - One folder per project (investigation)
    - Subfolders for each study (experiment)
    - and assay (measurement)
  - Date-based files folders (pairs well with lab notebook)



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Cataloging

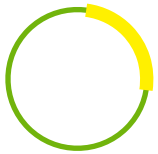
To connect lab knowledge and resources

Step 1

Which items want to be shared and cataloged?

Methods

Plant lines



Vectors

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Cataloging

To connect lab knowledge and resources

Step 1

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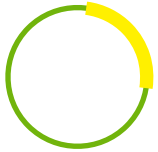
Create item database (catalog)

Name / ID items

Methods → MTHxxxxx

Plant lines → PLLxxxxx



Vectors → VECxxxxx

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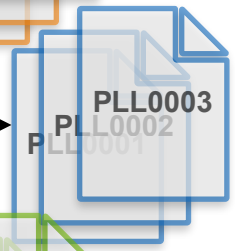

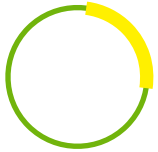

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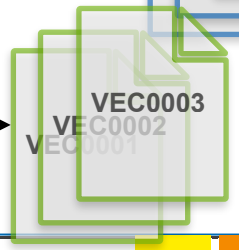

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Cataloging

To connect lab knowledge and resources

Curate and Version-control

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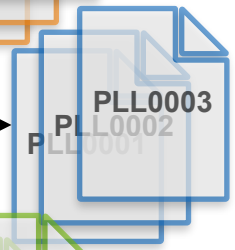
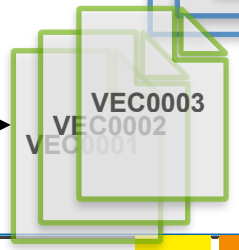


Vectors → VECxxxxx



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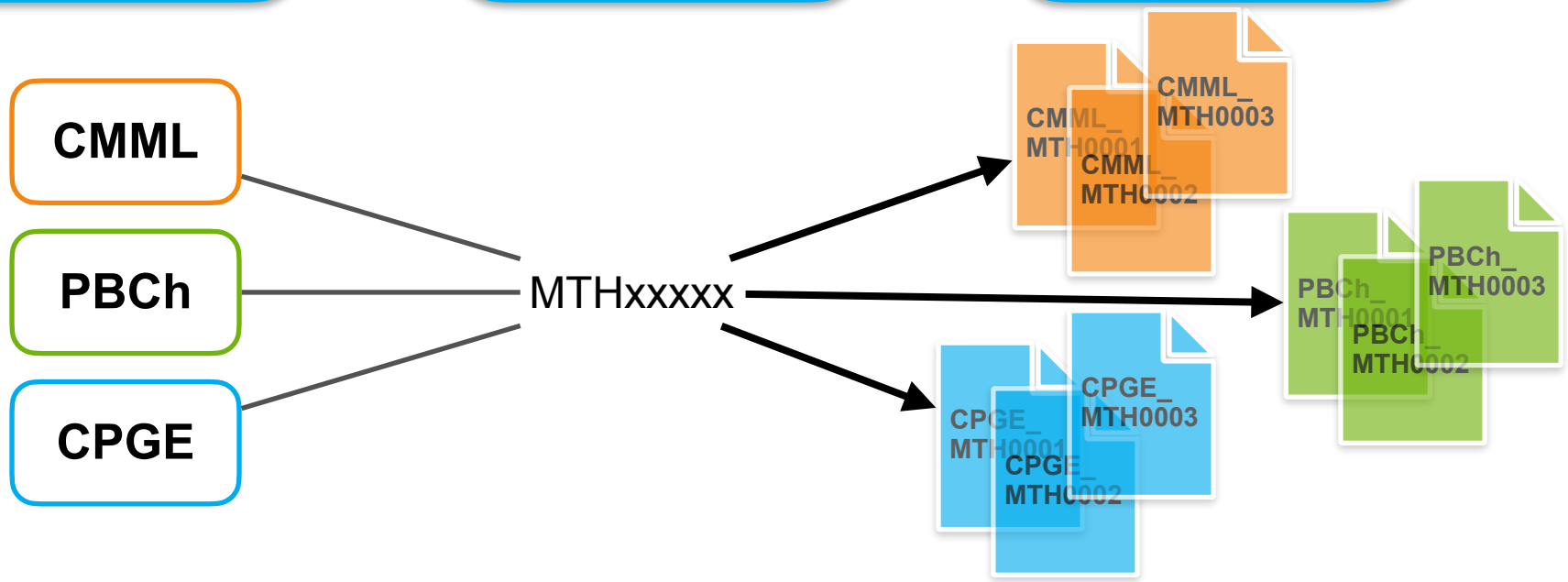

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The Weberlab database

The Weberlab database

- Adding a new item
  - Following the code and naming conventions
- Adding a new type of item
  - And import a list of items

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The Weberlab database

2020.12.08

Database list AG Weber Database Code

code	name
ASY	Assay
EQP	Equipment
INS	Instrument
MTH	Method
PLL	Plant line
PRJ	Project
PRM	Primer
SDY	Study
SOP	Standard Operating Procedure
VEC	Vector

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The Weberlab database

2020.12.08

Team Team

How to elabFTW

elabFTW -How To- Article Adding a new item to the database

1. If the type of item (e.g. primer, vector, method) exists follow the steps below. If the type does not exist, contact an admin and ask to add it following these instructions.
2. Go to the "DATABASE" (on top), and open the "database list" for the type of item you want to add.
3. Open / edit the database list and add the item starting with a consecutive ID in the first column and save.
4. Go to the "DATABASE" (on top) and create (top right corner) the respective type of item following the Naming conventions and rules for Database IDs

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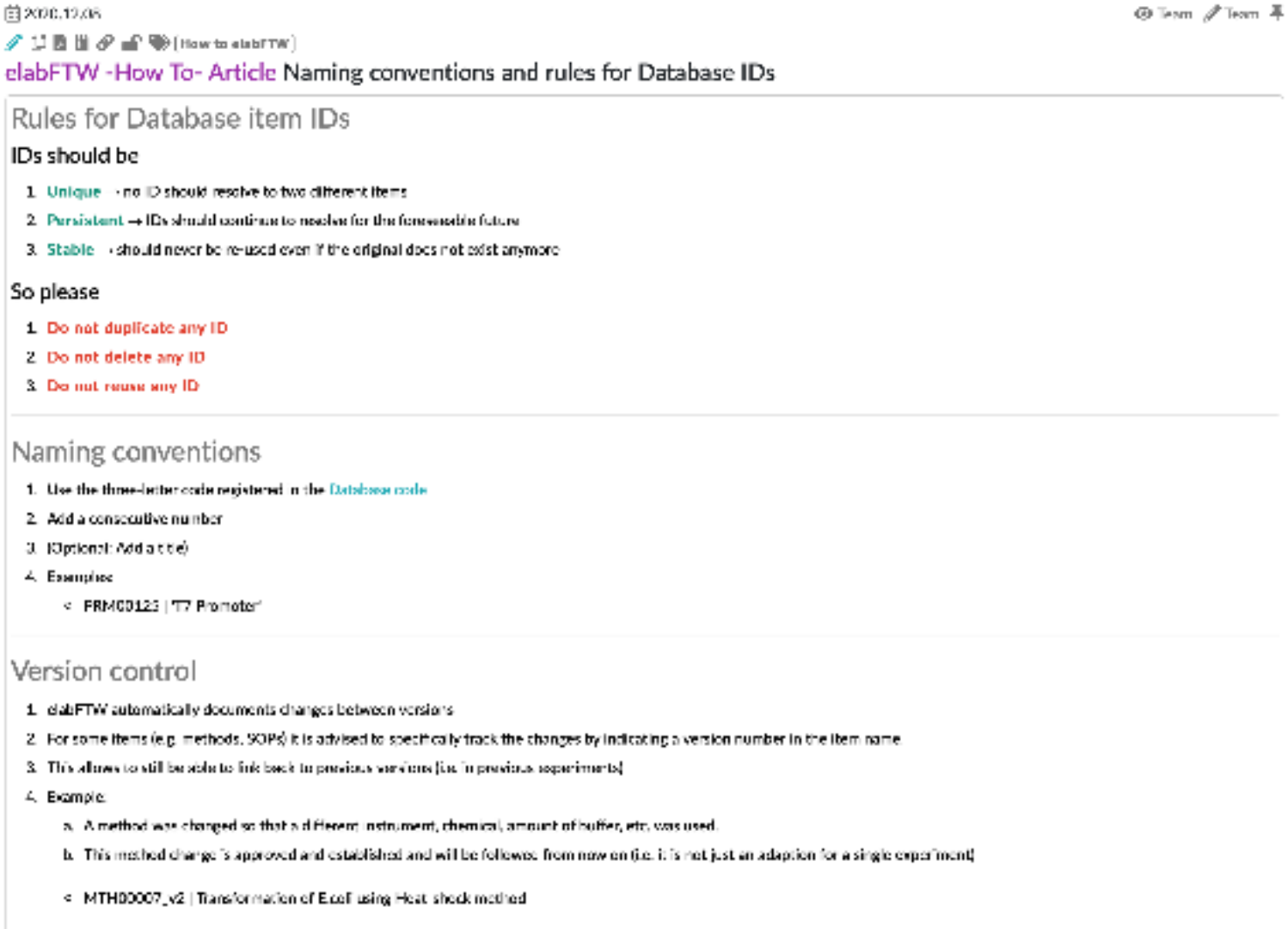
The Weberlab database



2020.12.08 — Team — Team

[How to elabFTW]

elabFTW -How To- Article Naming conventions and rules for Database IDs

Rules for Database item IDs

IDs should be

1. Unique - no ID should resolve to two different items
2. Persistent → IDs should continue to resolve for the foreseeable future
3. Stable - should never be re-used even if the original does not exist anymore

So please

1. Do not duplicate any ID
2. Do not delete any ID
3. Do not reuse any ID

Naming conventions

1. Use the three-letter code registered in the Database code
2. Add a consecutive number
3. (Optional: Add a title)
4. Examples
   - FRM00123 | "T7 Promoter"

Version control

1. elabFTW automatically documents changes between versions
2. For some items (e.g. methods, SOPs) it is advised to specifically track the changes by indicating a version number in the item name
3. This allows to still be able to link back to previous versions (i.e. in previous experiments)
4. Example:
   a. A method was changed so that a different instrument, chemical, amount of buffer, etc. was used.
   b. This modified change is approved and established and will be followed from now on (i.e. it is not just an adaption for a single experiment)
   - MTH00007_v2 | Transformation of E.coli using Heat shock method

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The Weberlab database

2020.12.08

How to elabFTW

elabFTW -How To- Article Adding a new item type to the database

As an admin:

1. Go to the "ADMIN PANEL" at the bottom
2. Go to the tab "TYPES OF ITEMS"
3. Add a meaningful "name" for the new item type.
4. (Recommended: Add a template scheme to describe the item)
5. Go to the "DATABASE" on top, create (top right corner) a table (as a "database list") to list all the items
6. The first column in the list should hold the IDs of the items
7. Add the code for the new item type to the AG Weber Database Code
8. If a list (e.g. excel table) for the type of item already exists, you can automatically import all items.
    a. Go to the "ADMIN PANEL" at the bottom.
    b. Follow the instructions in the the "IMPORT" tab

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elabFTW recommendations and responsibilities

elabFTW recommendations

- Tag experiments with investigation or study IDs
- Link database items in your experiments
- Follow the “ISA Model” to structure your projects
- Divide your *experiments* into sensible (sub) sections
  - Adapt status (Running - Success - Needs to be redone - Fail)
  - Use time-stamping at the end of an experiment!

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elabFTW recommendations II

- Regularly backup your data!
  - Export to ZIP
- Use a smart phone or tablet and save time
  - Check steps
  - Comment changes
  - Take pictures

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(Admin) Responsibilities

- Introduce new members to elabFTW

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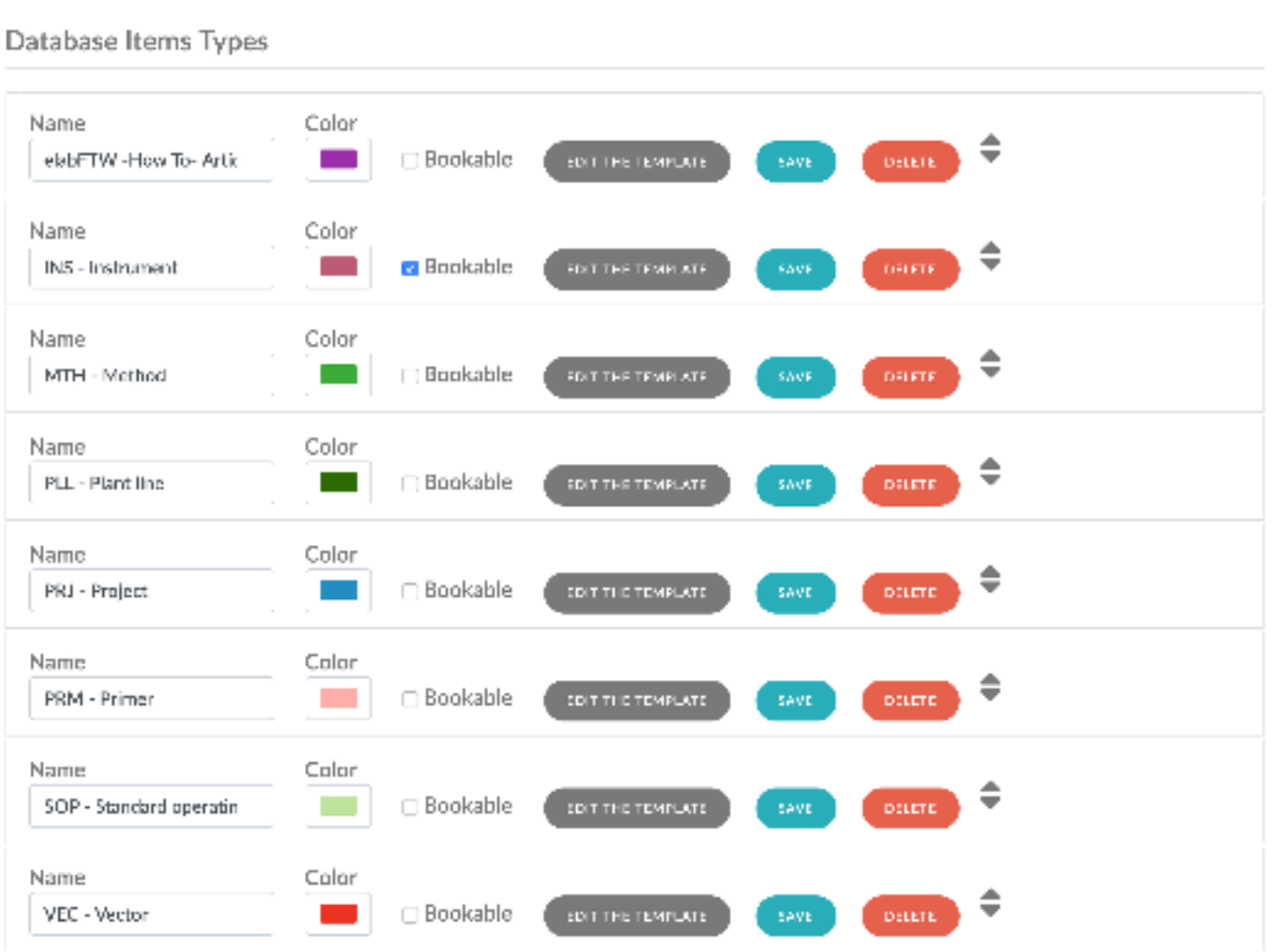
(Admin) Responsibilities

- Introduce new members to elabFTW
- Curate methods
- Manage
  - Groups
  - Types of items



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- Introduce new members to elabFTW
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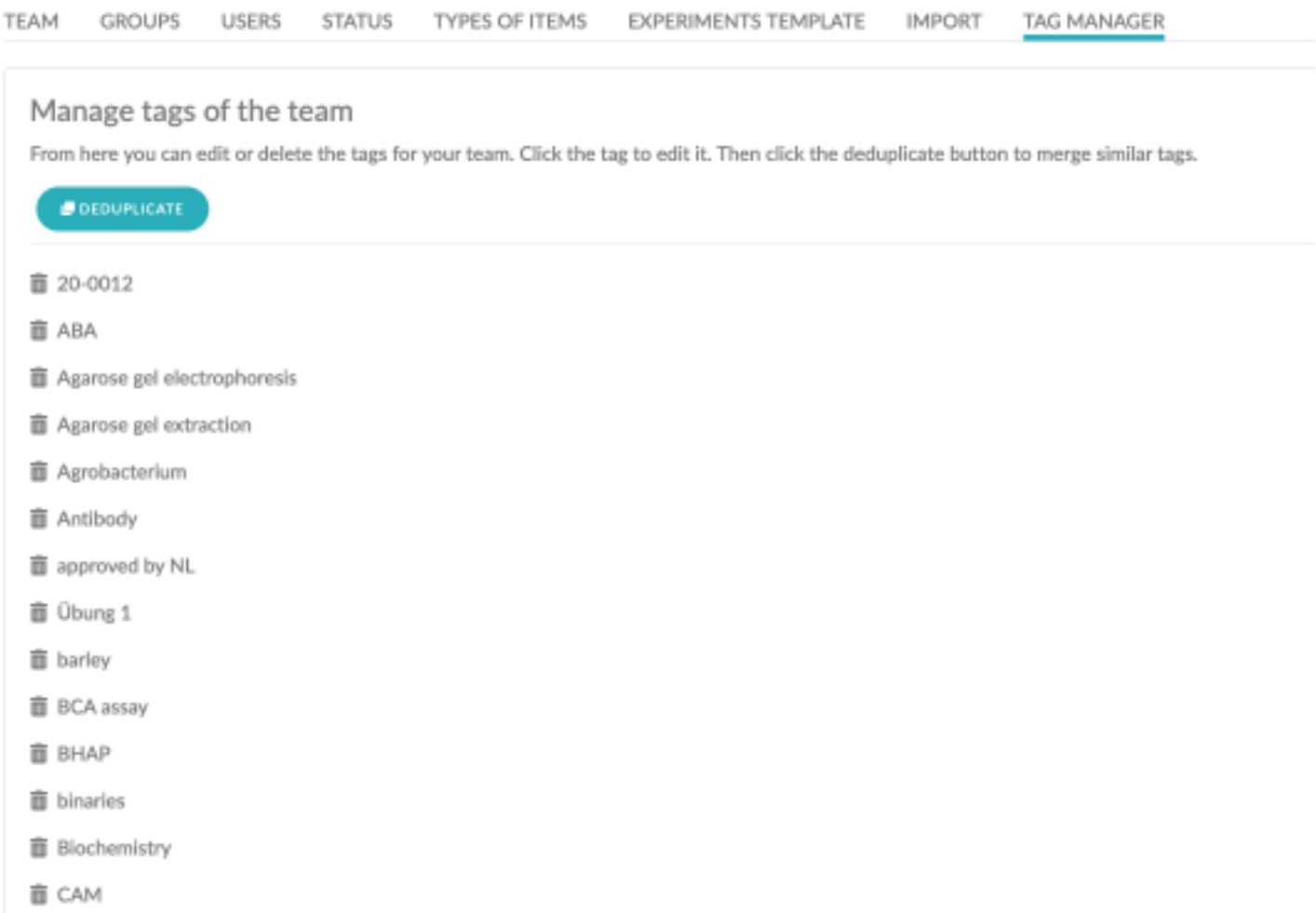
  - Tags



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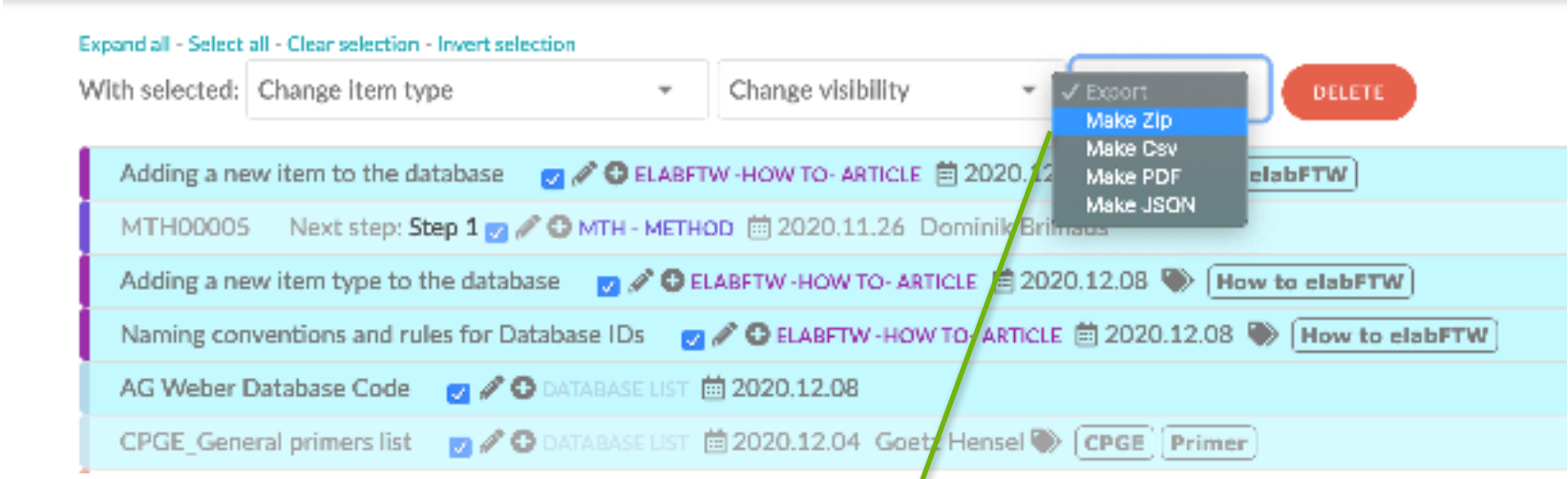
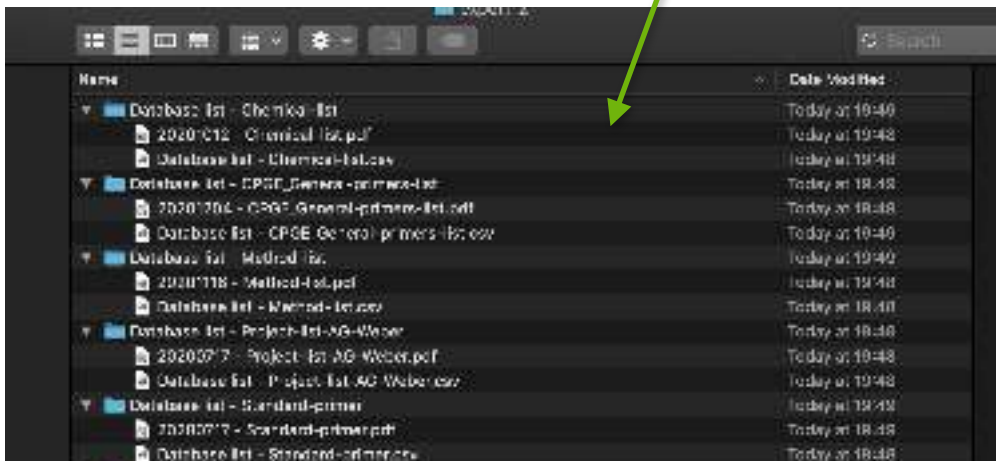




(User) Responsibilities

- Use it
  - Add experiments
  - Add items (following the rules)
- Comment on methods
- If an item type is missing, contact the admins.

Outlook

In collaboration with CRC1208, ZIM and other HHU members

- Share between HHU labs
  - Database for community-established schemes (item) templates
  - Resources (instruments, biological materials)
  - Knowledge (methods)

- Contact to Developer Nicolas Carpi (www.deltablot.com)

Outlook

Local

Curate and Version-control

Step 1

Which items want to be shared and cataloged?

Step 2

Create item database (catalog)

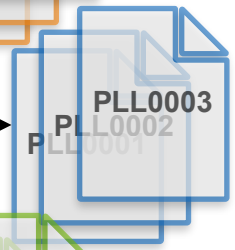
Name / ID items

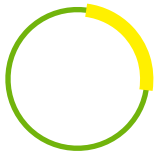
Step 3

Add items to database

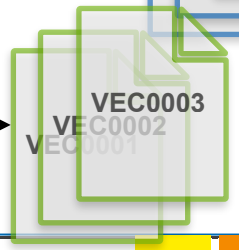
Methods → MTHxxxxx

Plant lines → PLLxxxxx





Vectors → VECxxxxx



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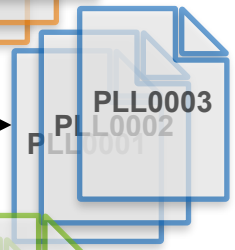
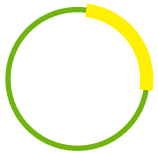
Using standard format

Standardized schemes / formats to describe items

Methods → MTHxxxxx

Plant lines → PLLxxxxx





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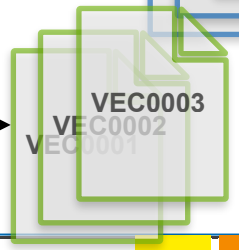

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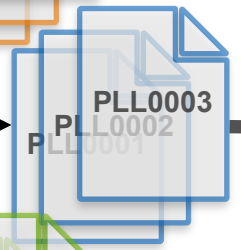

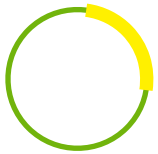

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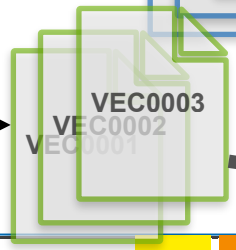

F A I R

Public registries

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Globally unique, stable, persistent identifiers (PIDs)

- Make data, digital objects, people, … uniquely identifiable
- See also
  - https://pidservices.org/
  - https://datacite.org
  - https://www.project-freya.eu/en

People

ORCID

Open Researcher and Contributor ID (https://orcid.org/)

Digital objects

doi

Digital Object Identifier (https://www.doi.org)

ePIC
Persistent Identifiers for eResearch

ePIC consortium (https://www.pidconsortium.net)

Resources

Research Resource IDentification

Research Resource Identifiers (https://www.rrids.org)

Institutions

ROR

Research Organization Registry (https://ror.org)

CEPLAS: https://ror.org/034waa237

GRID
Global Research Identifier Database

Global Research Identifier Database (https://grid.ac)

CEPLAS: https://grid.ac/institutes/grid.503026.2

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Your support contacts ;)

- Weberlab elabFTW Admins: **Nicole, Miguel, Götz, Philipp**
- Technical support: Nina Knipprath (https://www.fdm.hhu.de)
- Developing elabFTW @ HHU: Stephan Majda (https://www.sfb1208.hhu.de)
- Data management in general: Hajira Jabeen, Dominik Brilhaus (https://www.ceplas.eu)