

DataHUB

a two-day adventure to prepare your lab for the ARC universe

Dominik Brilhaus – CEPLAS Data Science June 28th, 2023

# **Annotated Research Context** (ARC)



# The ARC Club

Preparation

before August 16th, 2023

Dominik Brilhaus – CEPLAS Data Science

#### **Checklist hands-on sessions**

Please prepare the following before the workshop:

#### Required:

- Register at DataPLANT
- ✓ Install ARCitect on your computer
- ✓ Install Swate on your computer

#### Recommended (for trouble-shooting):

- ✓ Find your command line
- ✓ Install ARC Commander and dependencies on your computer
- ✓ Install VS Code

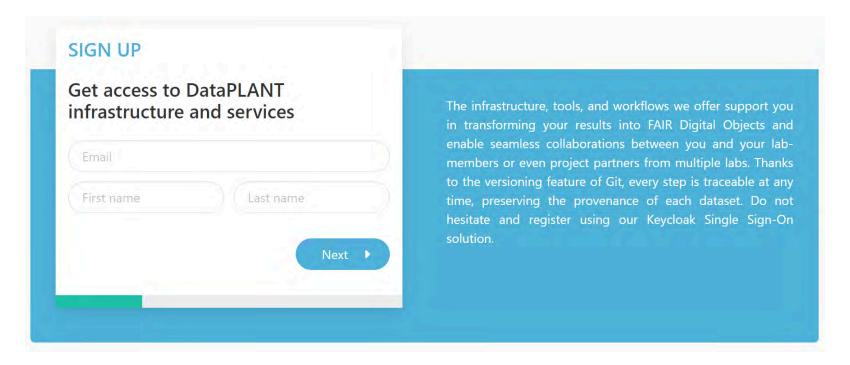






# **DataPLANT Registration**

If you do not have a DataPLANT account, please register at the DataPLANT website.



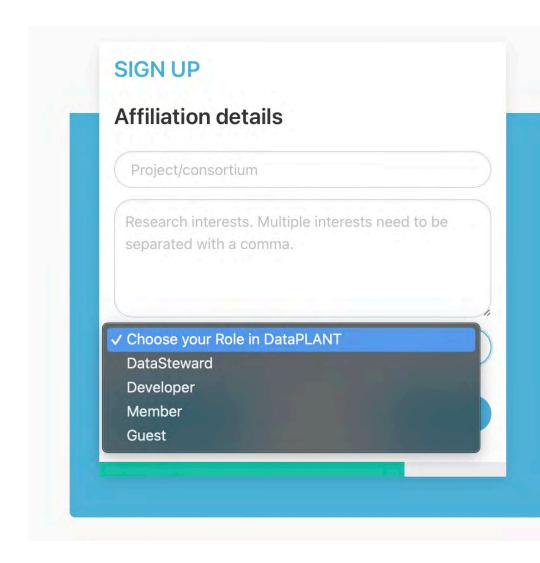






#### Role and consortium

Please add your Project/consortium (e.g. CEPLAS, SFB, TRR) and choose the role Guest









#### Join the group

Once signed-up and logged in, please join the HHU Plant Biochemistry group.







# **ARCitect Installation**

Please follow the instructions to install the latest version of ARCitect.

- macOS
- Windows







# **Swate Installation**

Please follow these instructions to install the latest version of Swate.







# Recommended for trouble-shooting

We will likely not use the tools on the next few slides.

However, as of now (early August 2023), it's probably better to have them ready for trouble-shooting and to show some inner workings of the ARC.







#### The command line

Find the **command-line interface (CLI)** on your system.

- On Windows: Enter powershell into the explorer path
- On MacOS: Search terminal via spotlight (第 + \_\_) or navigate to Applications -> Utilities -> Terminal

In our tutorials we sometimes use *terminal*, *command-line interface (CLI)* and *powershell* interchangeably.







#### **ARC Commander Installation**

Please install the latest version of the ARC Commander and dependencies for your operating system according to the manual's setup instructions.

Check if the ARC Commander is functional by displaying the ARC Commander version and help menu:

arc --version

#### Setup ~

**Installing Dependencies** 

**Configure Git** 

Installing the ARC Commander

Windows

MacOS

Linux

DataHUB Access

Before we start







#### Have a simple text editor ready

- Windows Notepad
- MacOS TextEdit

Recommended text editor with code highlighting, git support, terminal, etc: Visual Studio Code







#### Resources



#### **DataPLANT (nfdi4plants)**

Website: https://nfdi4plants.org/

Knowledge Base: https://nfdi4plants.org/nfdi4plants.knowledgebase/

DataHUB: https://git.nfdi4plants.org

GitHub: https://github.com/nfdi4plants







#### The ARC Club

Day 1 – Into the ARC

Dominik Brilhaus – CEPLAS Data Science

August 16th, 2023







# **ARC Club Goals**

- Move existing datasets into ARCs
- Share them via the DataHUB
- First few steps into ARCs
- Data users can pick them up from there







# Rules: perfect is the enemy of good

- There is no perfect ARC
- There is no complete ARC
- The only bad ARCs are those that don't exist yet.

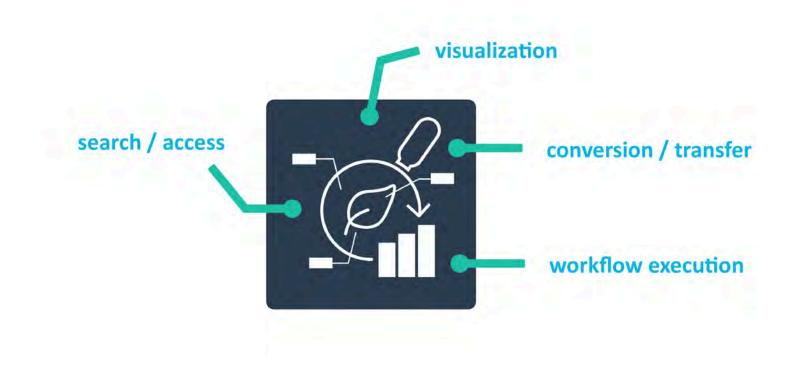
Let's get started, the rest is easy







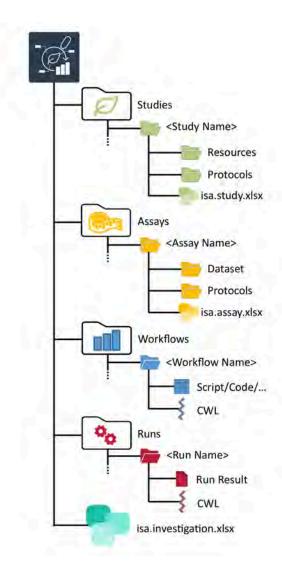
# **Annotated Research Context (ARC)**







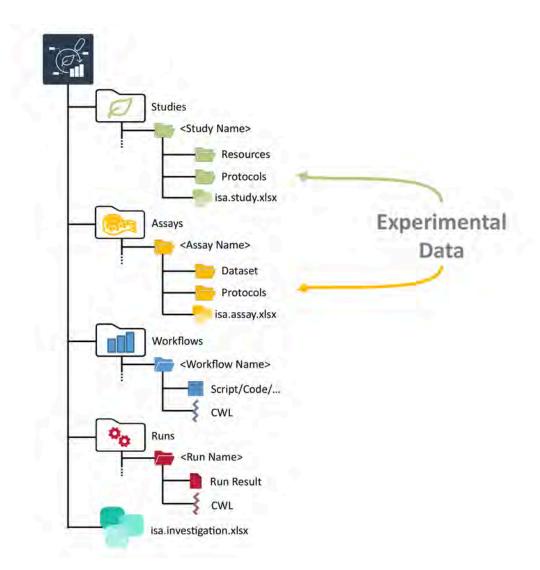








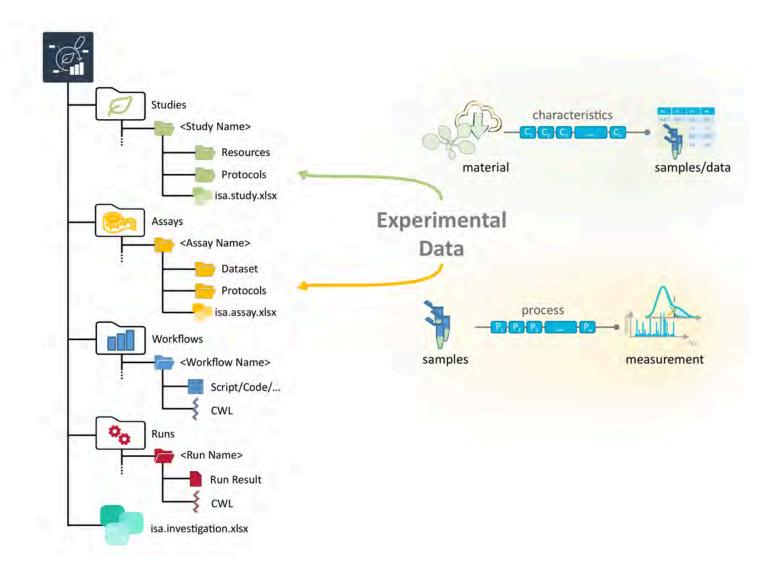








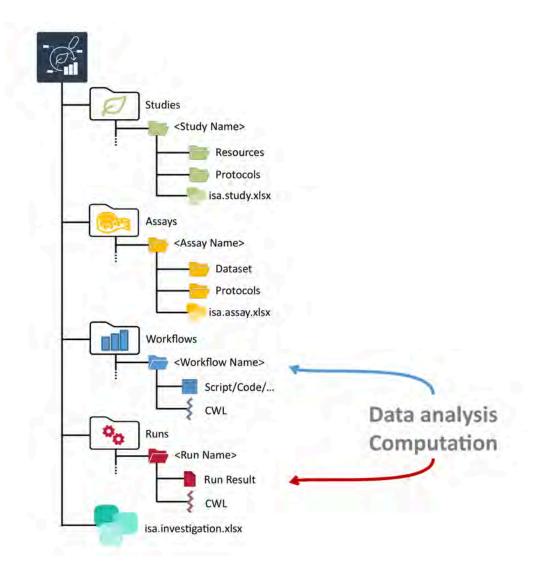








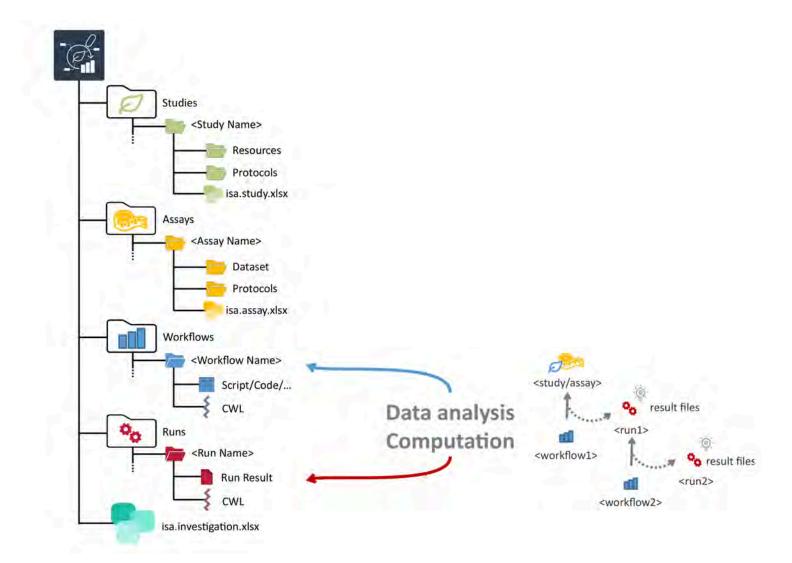








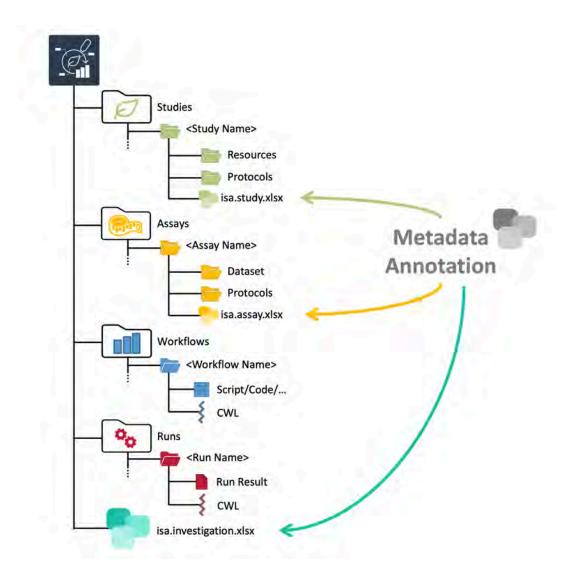
















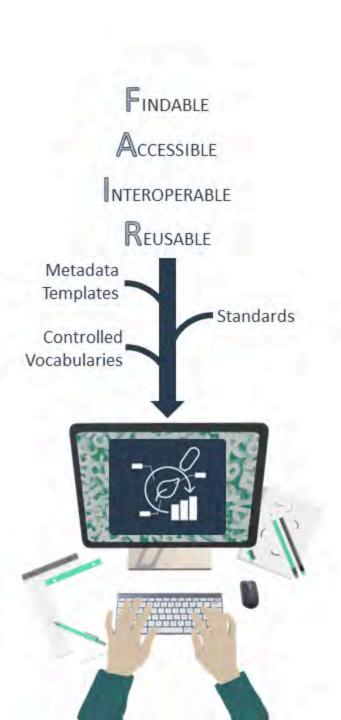




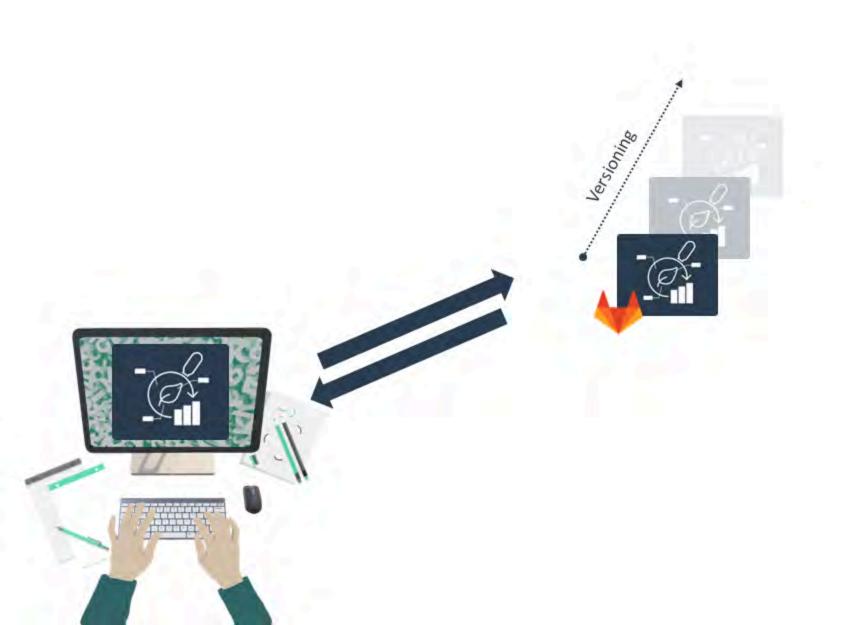








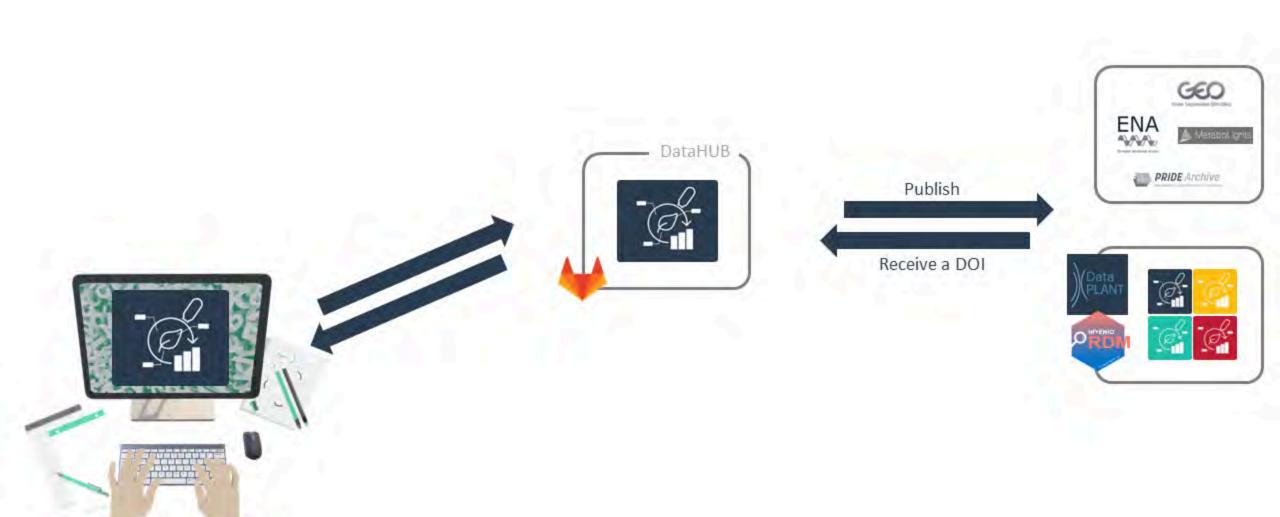


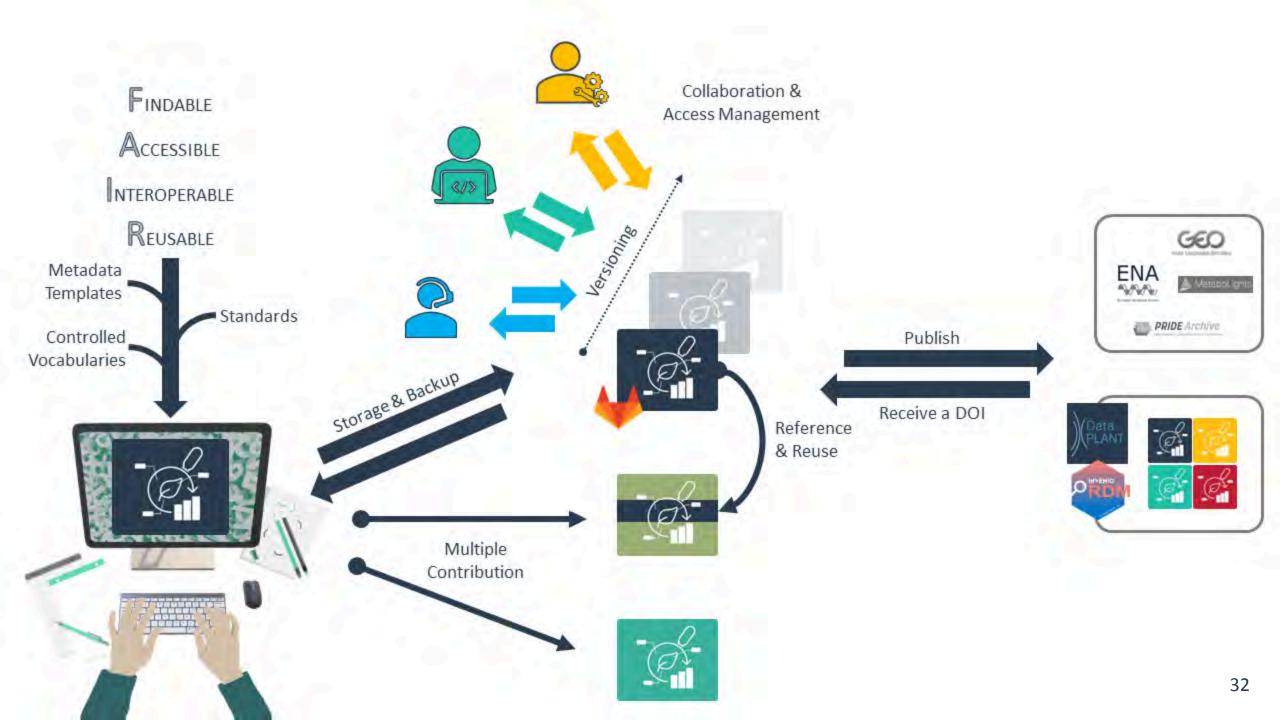












#### **Contributors**

Slides presented here include contributions by

- Dominik Brilhaus | GitHub | ORCID
- Cristina Martins Rodrigues | GitHub | ORCID
- Martin Kuhl | GitHub | ORCID







# The ARC Club

ARCitect QuickStart

Dominik Brilhaus – CEPLAS Data Science

August 16th, 2023

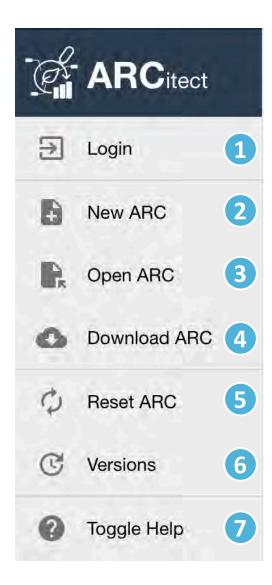






#### Initiate the ARC folder structure

- 1. Create a New ARC (2)
- 2. Select a location and name for your ARC









#### Your ARC's name

- By default, your ARC's name will be used
  - for the ARC folder on your machine
  - to create your ARC in the DataHUB at https://git.nfdi4plants.org/<YourUserName>/
     <YourARC> (see next steps)
  - as the identifier for your investigation
- Make sure that no ARC exists at https://git.nfdi4plants.org/<YourUserName>/<YourARC> . Otherwise you will sync to that ARC.



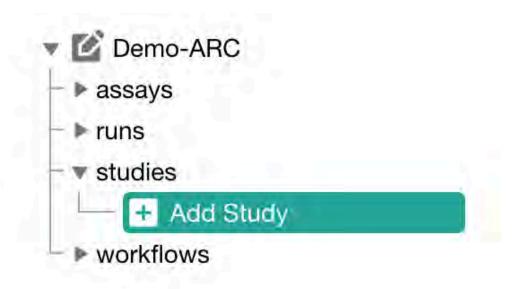






#### Add a study

by clicking "Add Study" and entering an identifier for your study





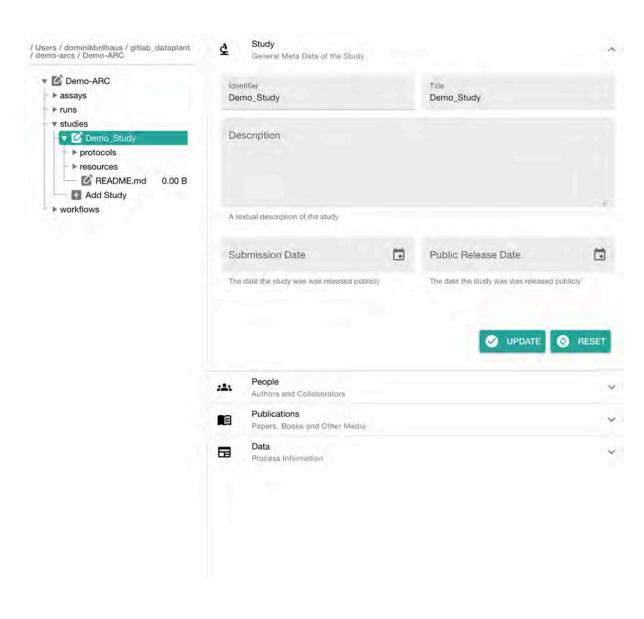




## Add information about your study

In the study panel you can add

- general metadata,
- people, and
- publications



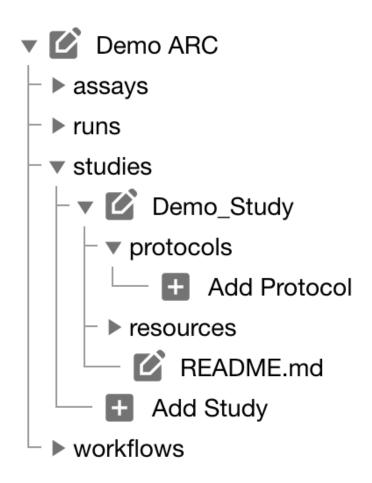






#### Add protocols to your study

In the file tree you can add protocols





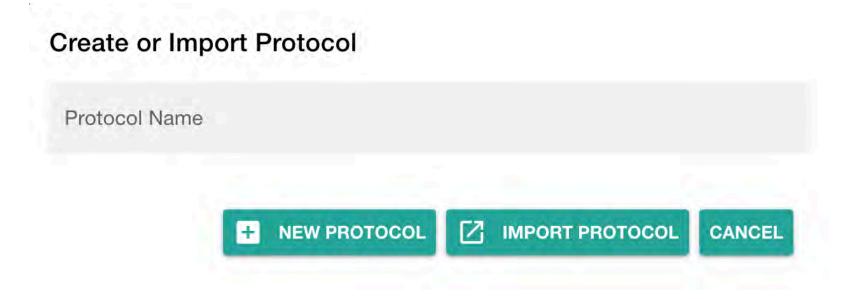




#### Add protocols

#### You can either

- directly write a **new protocol** within the ARCitect or
- import an existing one from your computer









#### Add an assay

by clicking "Add Assay" and entering an identifier for your assay





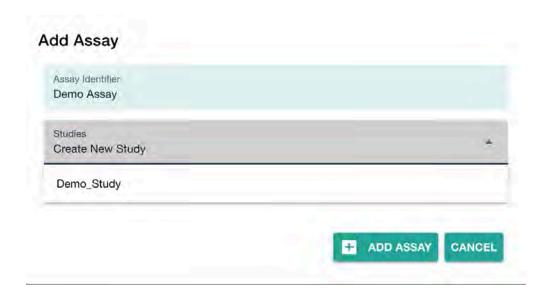




#### Link your assay to a study

#### You can either

- link your new assay to an existing study in your ARC or
- create a new one





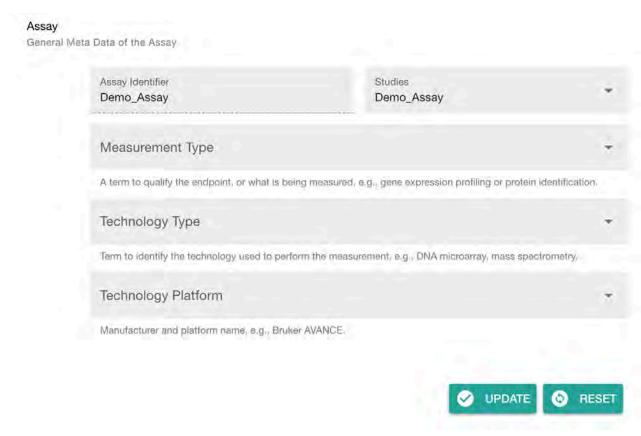




## Add information about your assay

In the assay panel you can

- 1. link or unlink the assay to studies, and
- 2. define the assay's
  - measurement type
  - technology type, and
  - technology platform.





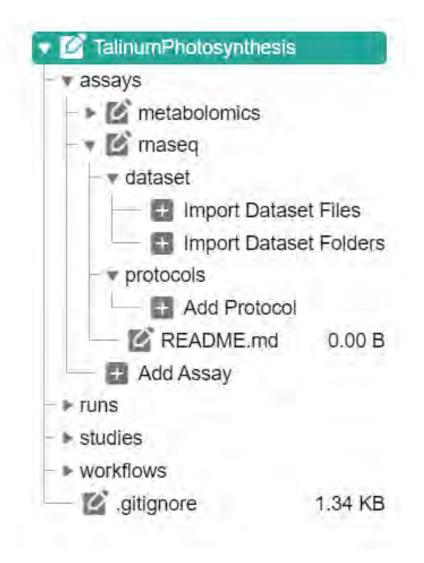




#### Add protocols and datasets

In the file tree you can

- add a dataset and
- protocols associated to that dataset.
- **Add Dataset** allows to import data from any location on your computer into the ARC.
- Depending on the file size, this may take a while. Test this with a small batch of files first.





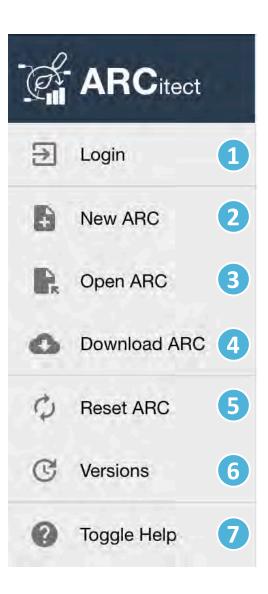




#### Login to the DataHUB

Click **Login** (1) in the sidebar to login to the DataHUB.

This automatically opens your browser at the DataHUB (https://git.nfdi4plants.org) and asks you to login, if you are not already logged in.



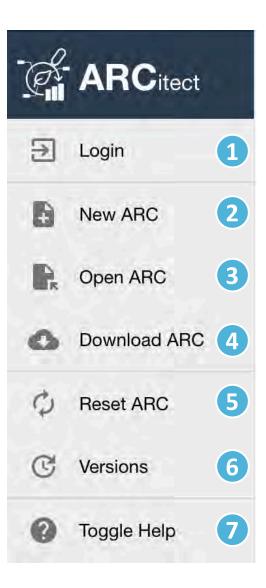






### Upload your local ARC to the DataHUB

From the sidebar, navigate to **Versions** (6)





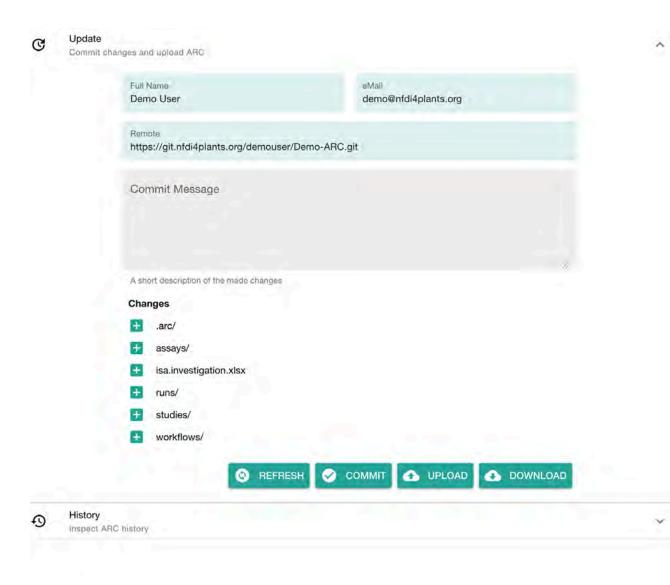




#### **Versions**

The versions panel allows you to

- store the local changes to your
   ARC in form of "commits",
- sync the changes to the DataHUB, and
- check the history of your ARC









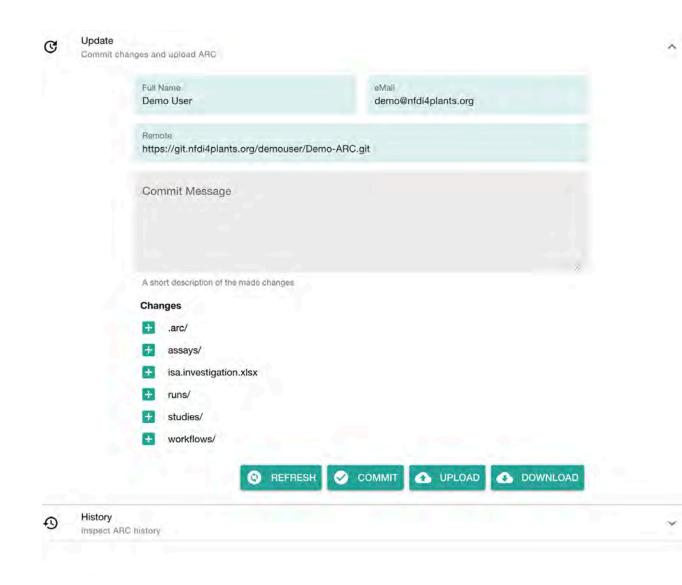
#### **Connection to the DataHUB**

If you are logged in, the versions panel shows

- your DataHUB's Full Name and eMail
- the URL of the current ARC in the DataHUB

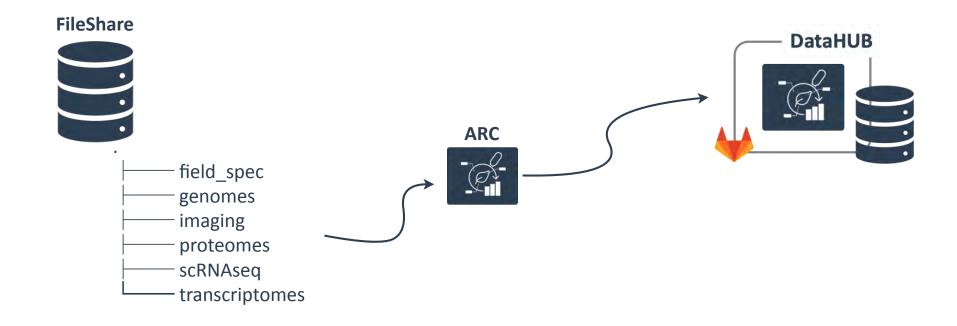
https://git.nfdi4plants.or
g/<YourUserName>/<YourARC>

#### The ARC Club





#### Moving from FileShare to DataHUB – via ARCs









#### **Assign projects**







#### Rough routine for each project

- 1. Identify the available data and resources
- 2. Create the ARC
- 3. Add metadata and data
- 4. Share via DataHUB group https://git.nfdi4plants.org/hhu-plant-biochemistry/







#### Low(er) hanging fruits: published projects

- 1. Add the authors
- 2. Add the publication(s)
  - i. Add citation and DOI
  - ii. Add supplemental
  - iii. Convert M&M to protocols
- 3. Reference data in public repositories
- 4. Add large data (e.g. from file share)
- 5. Set ARC to public!







#### **More challenging ARCs**

- (unpublished) left-overs of colleagues who have since moved
- unclear







#### Collect / derive as much info about the investigation as possible

#### **MUST** haves

```
Investigation Identifier
Investigation Title
Investigation Publication Status
Investigation Person Last Name
Investigation Person First Name
```

This and more investigation-level info can be collected in the ARC's

isa.investigation.xlsx







#### **Create and share the ARC**

```
arc init
arc sync -f -r https://git.nfdi4plants.org/hhu-plant-biochemistry/<InvestigationID>
```







#### Copy data

- 1. **Copy** data to the ARC, do not **move** data from original source (we'll take care of that later)
- 2. Ideally use rsync rather than copying manually
- 3. Ideally use md5 or md5sum to check for correct file transfer
- Ask the coders for help!







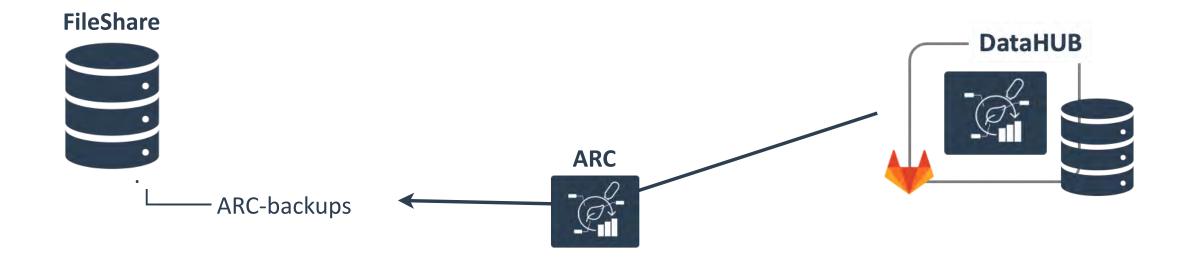
#### Perspective and administration in the future







#### **Administration / Backup**









#### The ARC Club

Intro and Hands-on Swate

Dominik Brilhaus – CEPLAS Data Science

August 17th, 2023







#### Goals

- Get familiar with ISA metadata and Swate
- Annotate data in your ARC







#### **Check Swate installation**

- ✓ Make sure Swate is installed:
  - 1. Open Excel (online or Desktop)
  - 2. Go to the Insert tab: Click the arrow next to "My Add-ins". There you should be able to select Swate.
  - 3. Go to the Data tab: you should see the Swate (Core) add-in.
- Paragraphy Alternatively, you can use Swate standalone
- ( this is however work in progress and likely to change)







#### Have a simple text editor ready

- Windows Notepad
- MacOS TextEdit

Recommended text editors with code highlighting:

Visual Studio Code https://code.visualstudio.com/







#### Download the demo data

git clone "https://demo-user:5ehDYeHcqP2MqVXsNNPu@git.nfdi4plants.org/teaching/demo-arc\_level1.git"





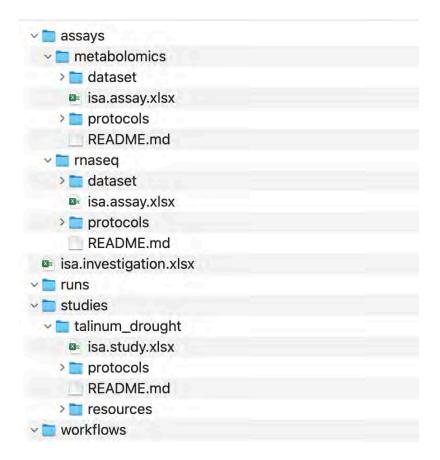


#### Where we left off last time

- Initiated an ARC
- Structured and ...
- Shared with collaborators

**Today** we want to











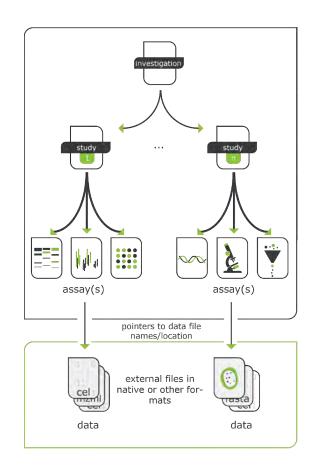
#### **Intro ISA**







#### **ARC** builds on ISA



#### Investigation

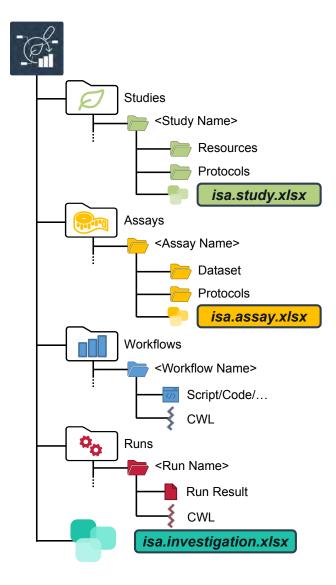
Overall goals
Scientific context

#### Study

Experimental design

#### **Assay**

Leading to (raw) data

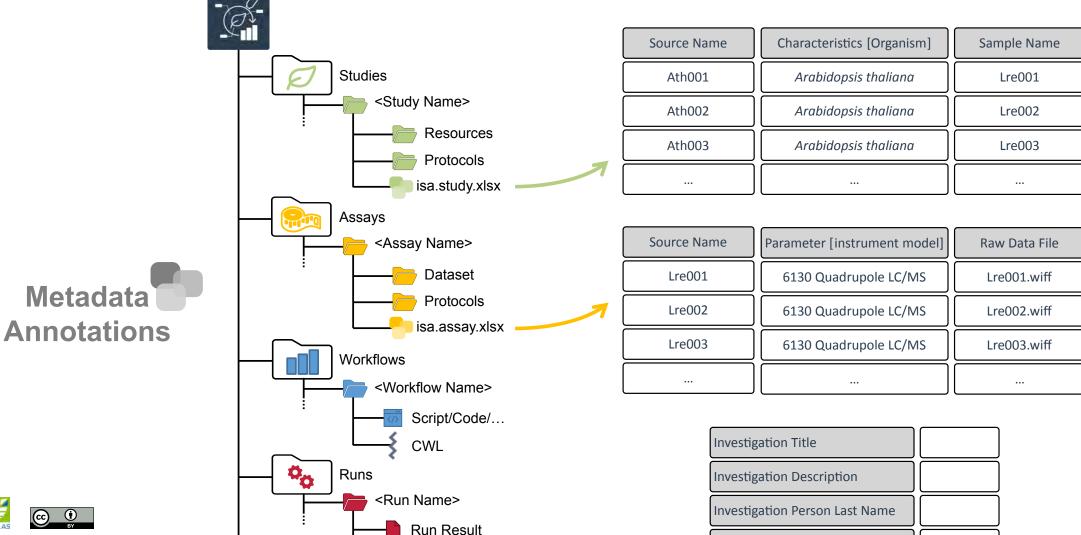








#### **ARC** builds on ISA



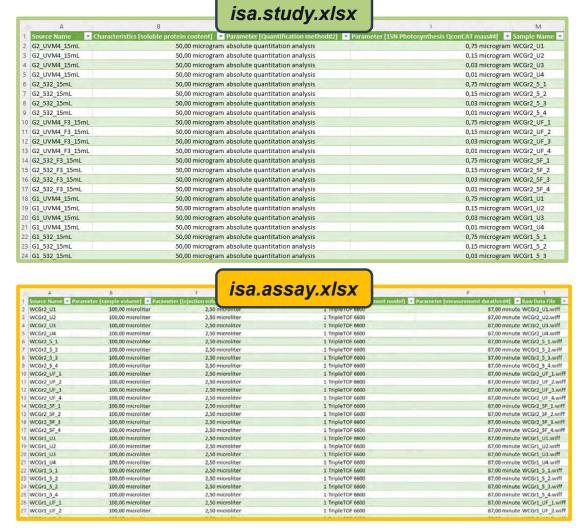






#### isa.<>.xlsx files within ARCs



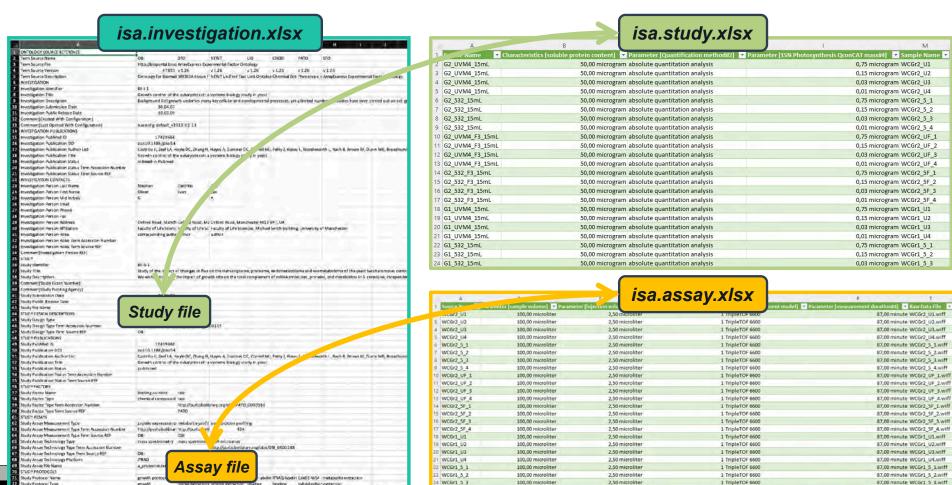






# Study and assay files are registered in the investigation file

http://purl.pholibrary.org/cbc/061 516



WCGr1 5 4

100,00 microlites

2,50 microlite

1 TripleTOF 6600

87,00 minute WCGr1 5 4.wiff



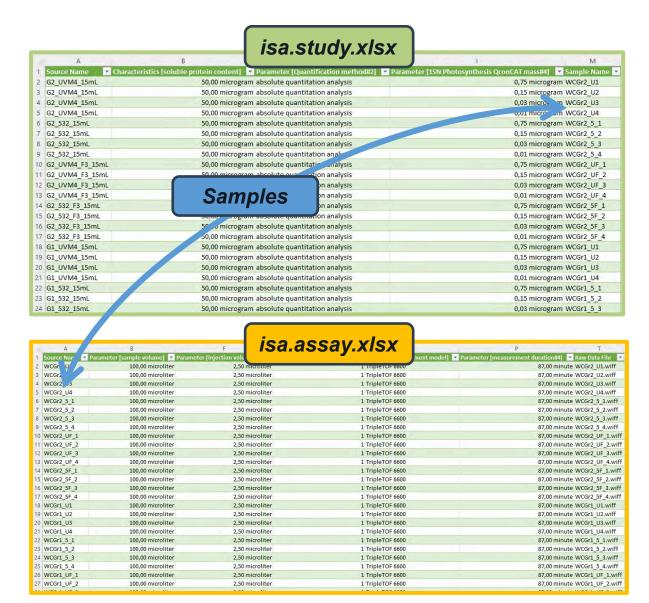




# The output of a study or assay file can function as input for a new isa.assay.xlsx

#### Output building blocks:

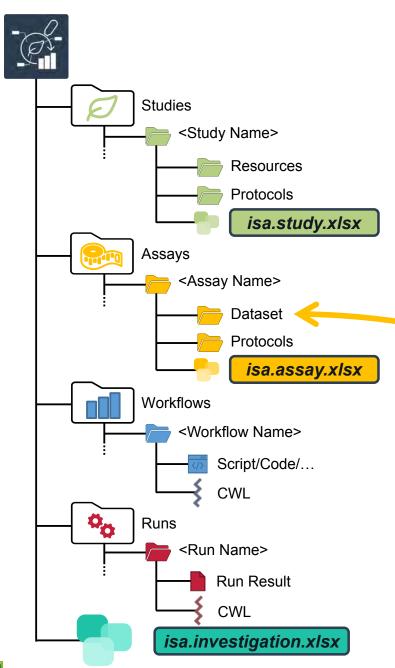
- Sample Name
- Raw Data File
- Derived Data File

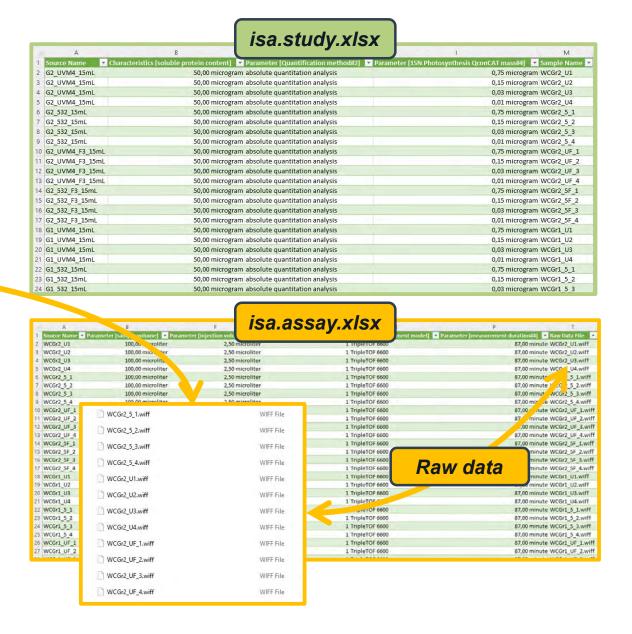


















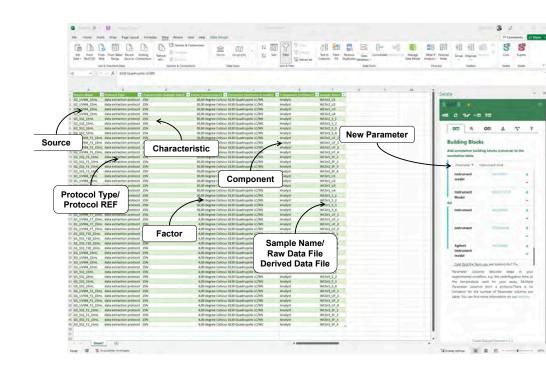
# **Annotation Building Block types**

- Source Name (Input)
- Protocol Columns
  - Protocol Type, Protocol Ref
- Characteristic
- Parameter
- Factor
- Component
- Output Columns
  - Sample Name, Raw Data File, Derived









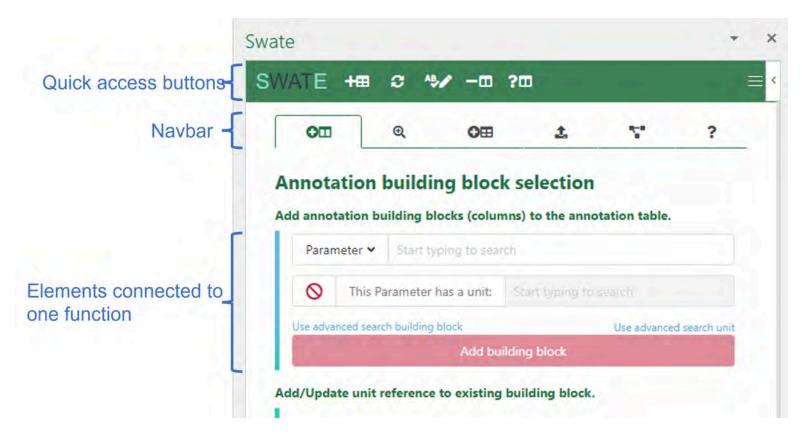
# Swate hands-on with demo data







### **Swate Overview**



Major areas of the Swate user interface.







### Let's annotate the plant samples first

- 1. Navigate to the demo ARC.
- 2. Open the lab notes studies/talinum\_drought/protocols/plant\_material.txt in a text editor.
- 3. Open the empty studies/talinum\_drought/isa.study.xlsx workbook in Excel.

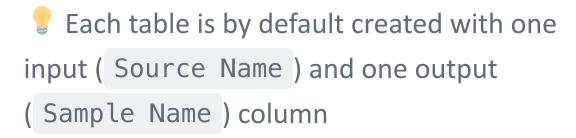




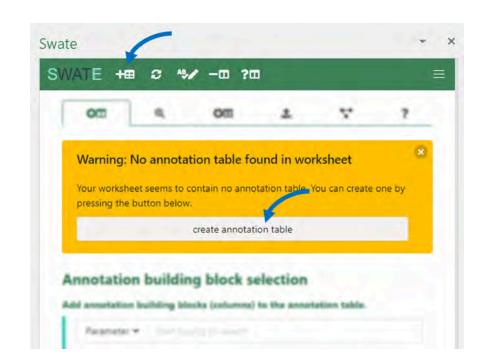


### Create an annotation table

Create a Swate annotation table via the create annotation table button in the yellow pop-up box *OR* click the Create Annotation Table quick access button.



Only one annotation table can be added per Excel sheet



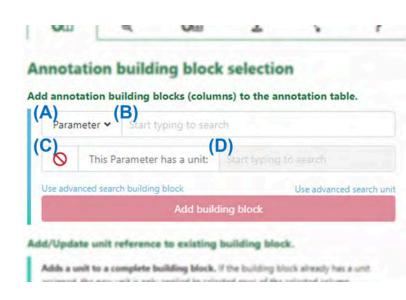






### Add a building block

- 1. Navigate to the *Building Blocks* tab via the navbar. Here you can add *Building Blocks* to the table.
- 2. Instead of *Parameter* select *Characteristic* from the drop-down menu (A)
- 3. Search for organism in the search bar (B). This search looks for suitable *Terms* in our *Ontology* database.
- 4. Select the Term with the id OBI:0100026 and,
- 5. Click Add building block.
- This adds three columns to your table, one visible and **two** hidden.









### Insert values to annotate your data

- 1. Navigate to the *Terms* tab in the Navbar
- 2. In the annotation table, select any number of cells below Characteristic [organism]
- 3. Click into the search field in Swate.
  - You should see organism showing in a field in front of the search field
- The search will now yield results related to organism
- 4. In the search field, search for "Talinum fruticosum"
- 5. Select the first hit and click | Fill selected cells with this term







### Add a building block with a unit

- 1. In the *Building Blocks* tab, select *Parameter*, search for light intensity exposure and select the term with id PECO:0007224.
- 2. Check the box for *This Parameter has a unit* and search for microeinstein per square meter per second in the adjacent search bar.
- 3. Select U0:0000160.
- 4. Click Add building block.
  - This adds four columns to your table, one visible and three hidden.







### Insert unit-values to annotate your data

In the annotation table, select any cell below Parameter [light intensity exposure] and add "425" as light intensity.

You can see the numbers being complemented with the chosen unit, e.g. 425.00 microeinstein per square meter per second







### Showing ontology reference columns

Hold Ctrl and click the *Autoformat Table* quick access button to adjust column widths and un-hide all hidden columns.

You can see that your organism of choice was added with id and source Ontology in the reference (hidden) columns.

1 This feature is currently not supported on MacOS







### **Update ontology reference columns**

Click the Update Ontology Terms quick access buttons.

This updates all reference columns according to the main column. In this case the reference columns for Parameter [light intensity exposure] are updated with the id and source ontology of the microeinstein per square meter per second unit.

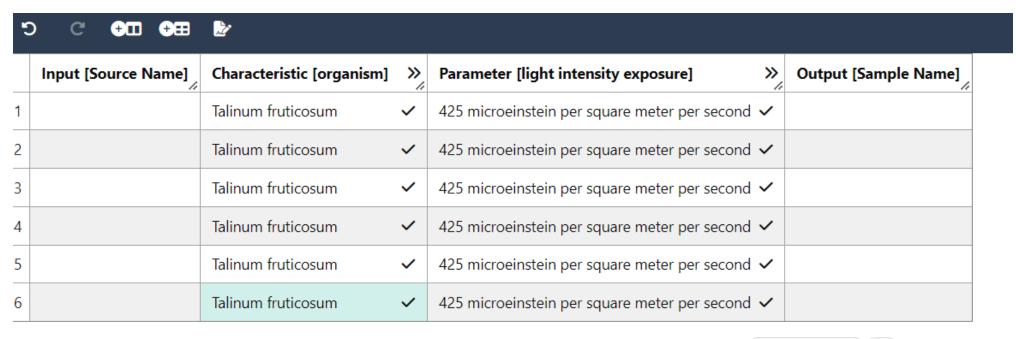






### Your ISA table is growing

At this point. Your table should look similar to this:











## **Hiding ontology reference columns**

Click the Autoformat Table quick access button without holding Ctrl to hide all reference columns.







## **Exercise**

Try to add suitable *building blocks* for other pieces of metadata from the plant growth protocol (studies/talinum\_drought/protocols/plant\_material.txt).







### Let's annotate the RNA Seq data

- 1. Navigate to the demo ARC.
- 2. Open the lab notes assays/rnaseq/protocols/RNA\_extraction.txt in a text editor.
- 3. Open the empty assays/rnaseq/isa.assay.xlsx) workbook in Excel.

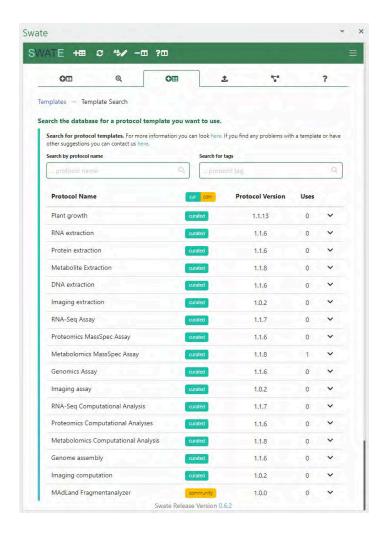






## Use a template

- 1. Navigate to *Templates* in the Navbar and click *Browse* database in the first function block.
- Here you can find community created workflow annotation templates
- 1. Search for RNA extraction and click select
  - You will see a preview of all building blocks which are part of this template.
- 2. Click Add template to add all Building Blocks from the template to your table, which do not exist yet.









## Adding / Updating unit references

Sometimes you need to add or update the unit of an existing building block.

- 1. Select any number of rows of the Parameter [biosource amount] building block to mark it for the next steps.
- 2. Open the Building Blocks tab
- 3. In the bottom panel "Add/Update unit reference to existing building block", search for the unit "milligram". Select the unit term and click Update unit for cells .
  - If you already had values in the main column they will be updated automatically.
- 4. Click the *Update Ontology Terms* quick access button, to update the reference columns.







### Remove building blocks

If there are any Building Blocks which do not fit your experiment you can use the Remove Building Block quick access button to remove it including all related (hidden) reference columns.

⚠ Due to the hidden reference columns, we recommend not to delete table columns via usual Excel functions.







### New process, new worksheet

- 1. Add a new sheet to the assays/rnaseq/isa.assay.xlsx) workbook.
- 2. Add the template "RNASeq Assay"







## **Exercise**

Try to fill the two sheets with the protocol details:

- assays/rnaseq/protocols/RNA\_extraction.txt and
- assays/rnaseq/protocols/Illumina\_libraries.txt







# Your ISA table is ready 🎉

Go ahead, adjust the Building Blocks you want to use to describe your experiment as you see fit.

Insert values using Swate Term search and add input and output.







### A small detour on "Excel Tables"

Swate uses Excel's "table" feature to annotate workflows. Each table represents one *process* from input (e.g. plant leaf material) to output (e.g. leaf extract).

Example workflows with three *processes* each:

- Plant growth → sampling → extraction
- Measured data files → statistical analysis → result files

Excel tables allow to group data that belongs together inside one sheet. This is not to be confused with a (work)sheet or workbook.







### **Contributors**

Slides presented here include contributions by

- Dominik Brilhaus | GitHub | ORCID
- Kevin Frey | GitHub | ORCID
- Martin Kuhl | GitHub | ORCID











