



CEPLAS

Cluster of Excellence on Plant Sciences

ARCify your research project

October, 2024

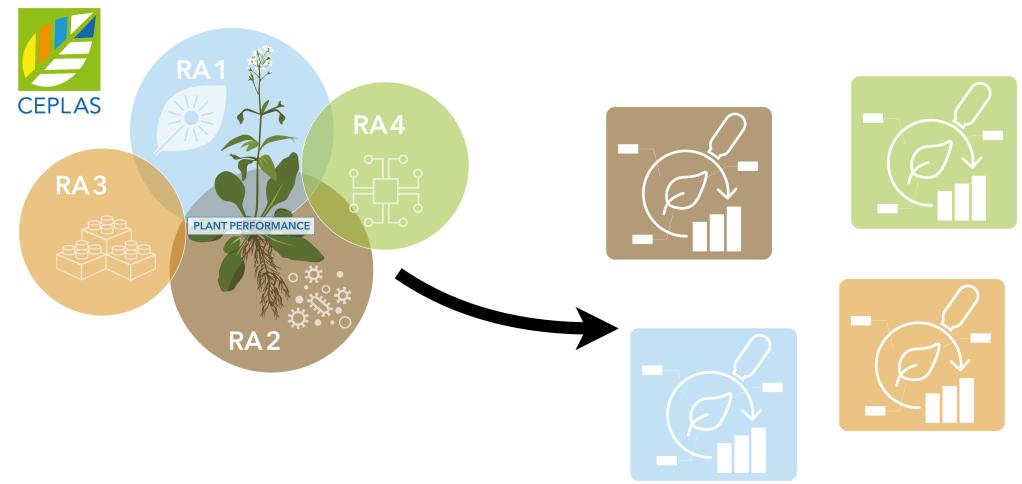
Dominik Brilhaus (CEPLAS)

Sabrina Zander (MibiNet)



Goals

- First few steps into ARC ecosystem
- Move existing datasets into ARCs
- Share them via the DataHUB
- Annotate with metadata



House-keeping

- Use the pad to raise questions and feedback
- Copy / paste links (hands-on)



Training Materials

Slides are shared via [DataPLANT knowledge base](#)

Resources – join the open source movement



DataPLANT (nfdi4plants)

DataPLANT Website: <https://nfdi4plants.org/>

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

DataHUB: <https://git.nfdi4plants.org>

GitHub: <https://github.com/nfdi4plants>

HelpDesk: <https://helpdesk.nfdi4plants.org>

You can help us by raising issues, bugs, ideas...

NEW! ARC website: <https://arc-rdm.org>

Continuous support

Data managers in Düsseldorf, Cologne, Jülich and close by (CEPLAS, MibiNet, TRR341) offer support.

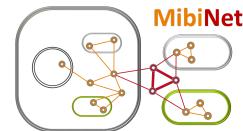
1. Slack Workspace for ad hoc support
2. Monthly user meeting (2nd Friday of the month)

→ [Details](#).



trr_341

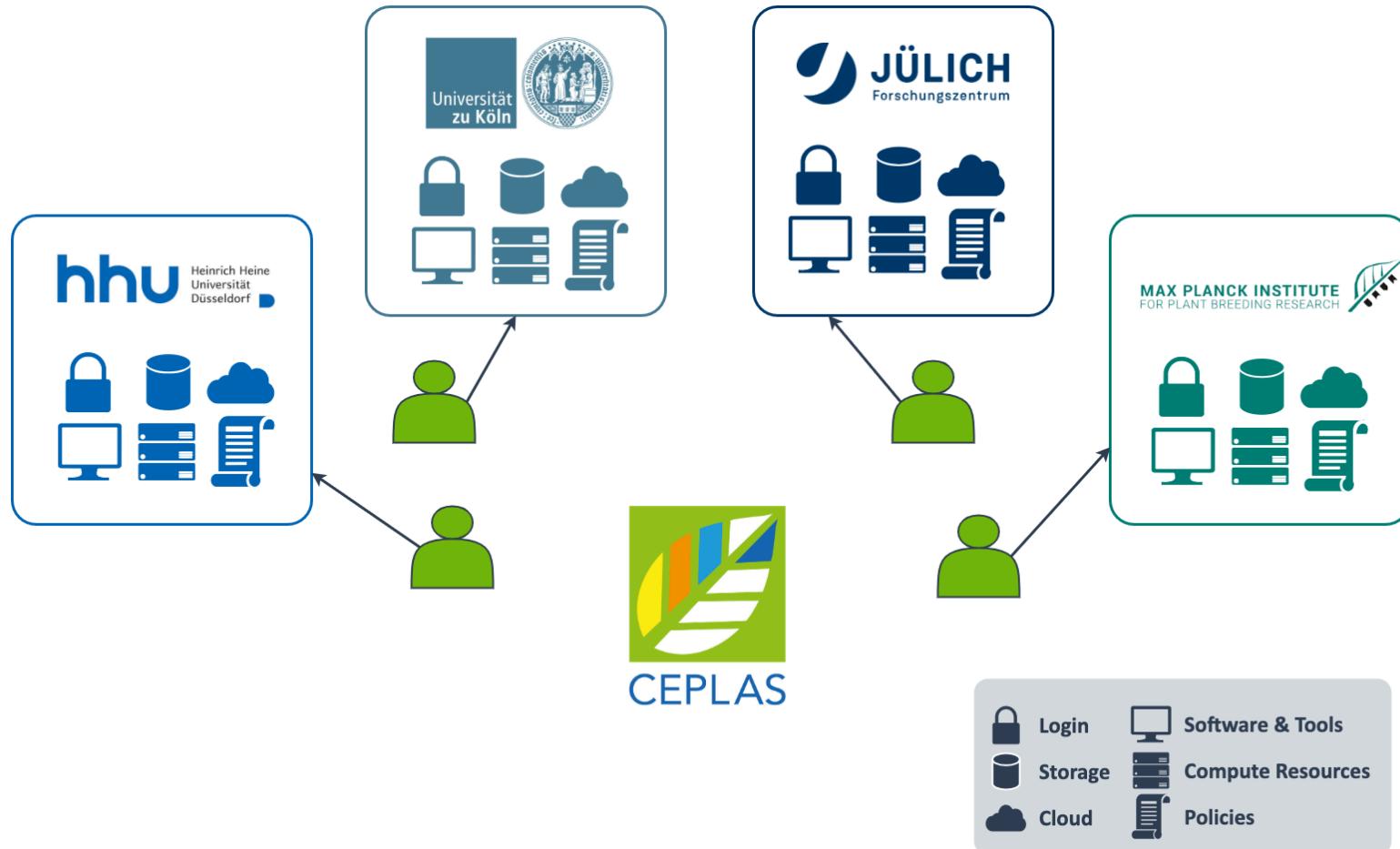
plant
ecological
genetics



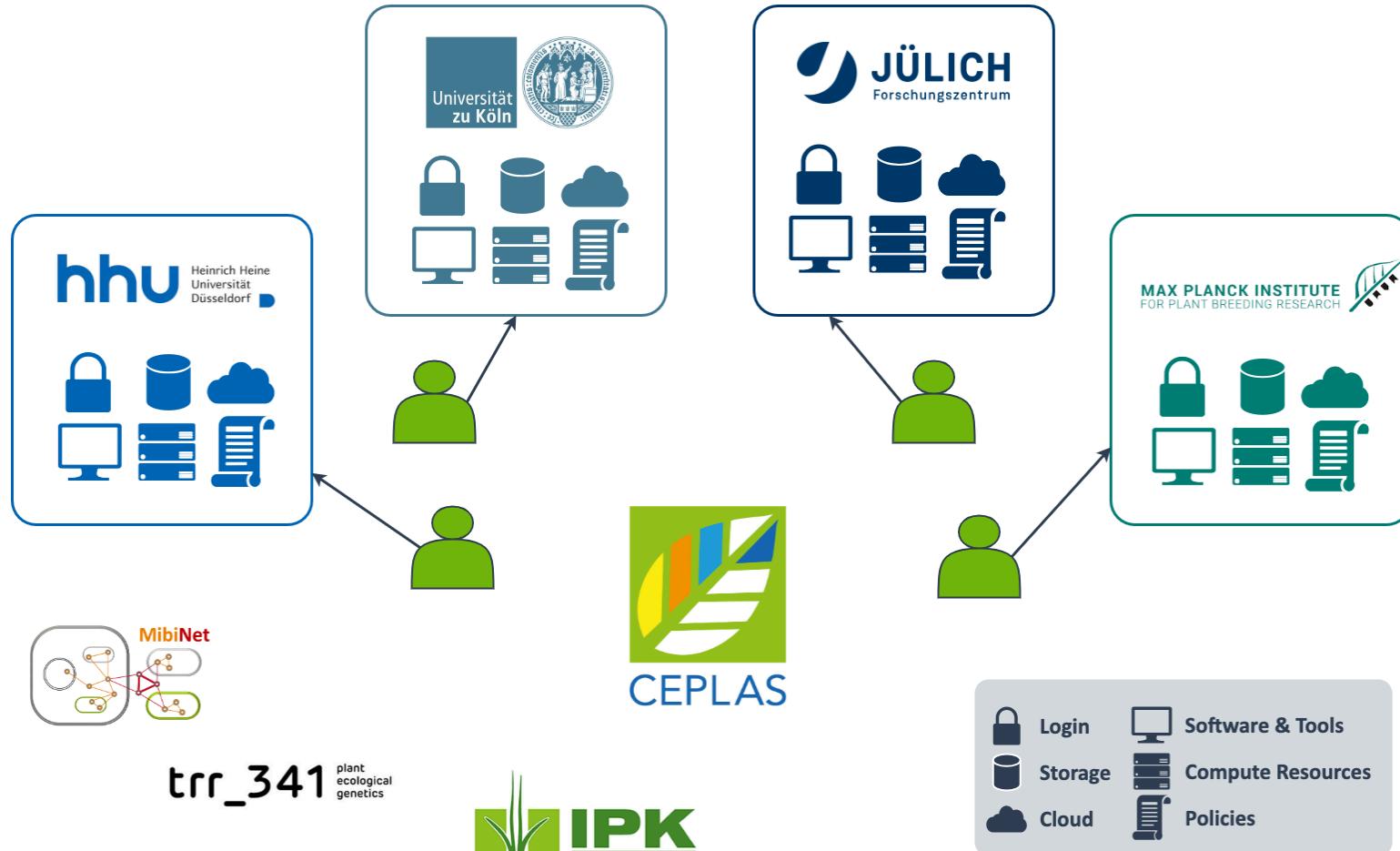
CEPLAS – One cluster, four locations



Data silos impede collaboration

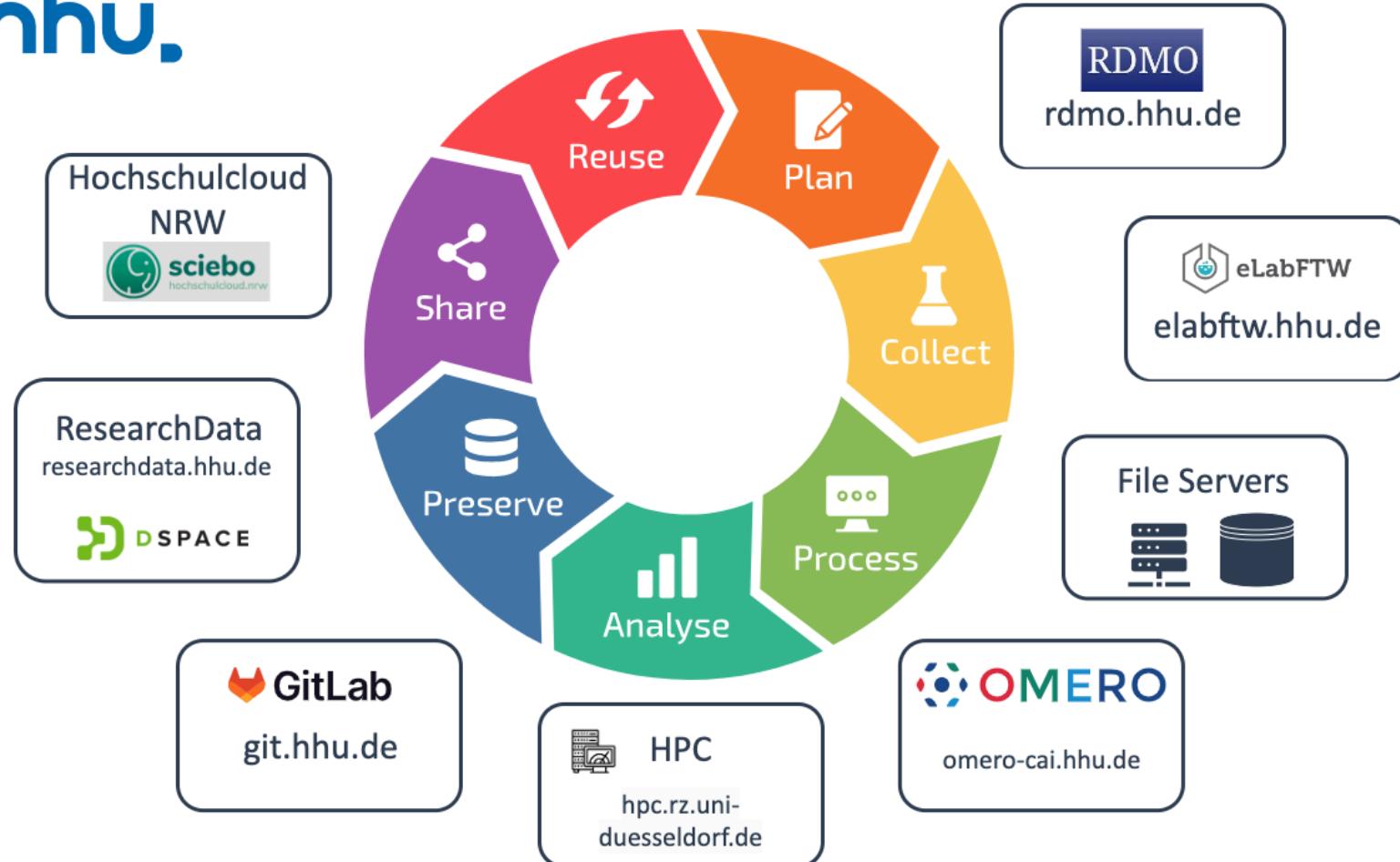


Data silos impede collaboration



Missing interfaces impede collaboration

hhu.



Data Stewardship between DataPLANT and the community

Community



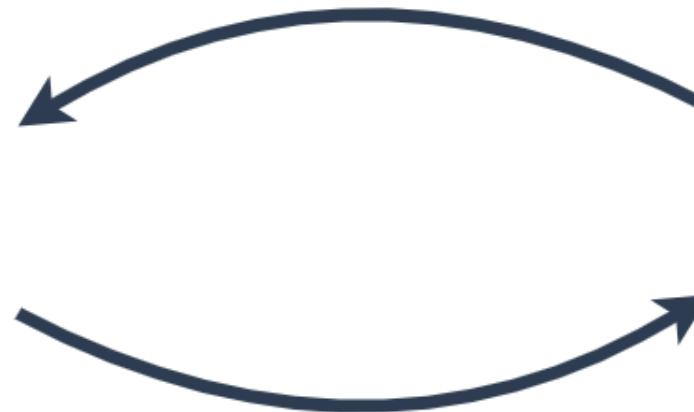
CEPLAS

Domain experts
User experience
Training

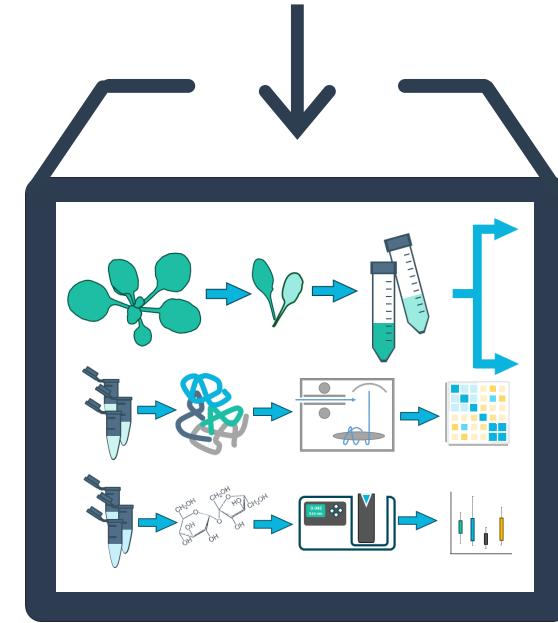
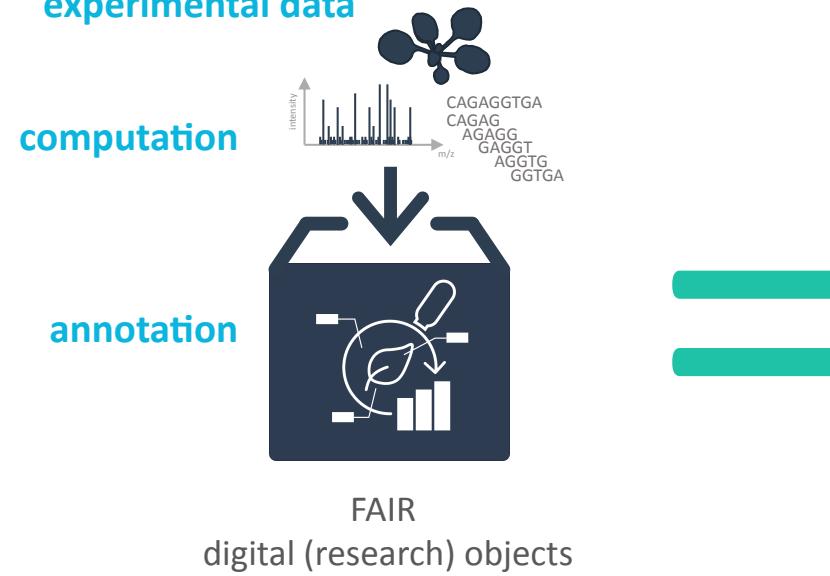
nfdi4plants



Service provider
Developers
Tech experts

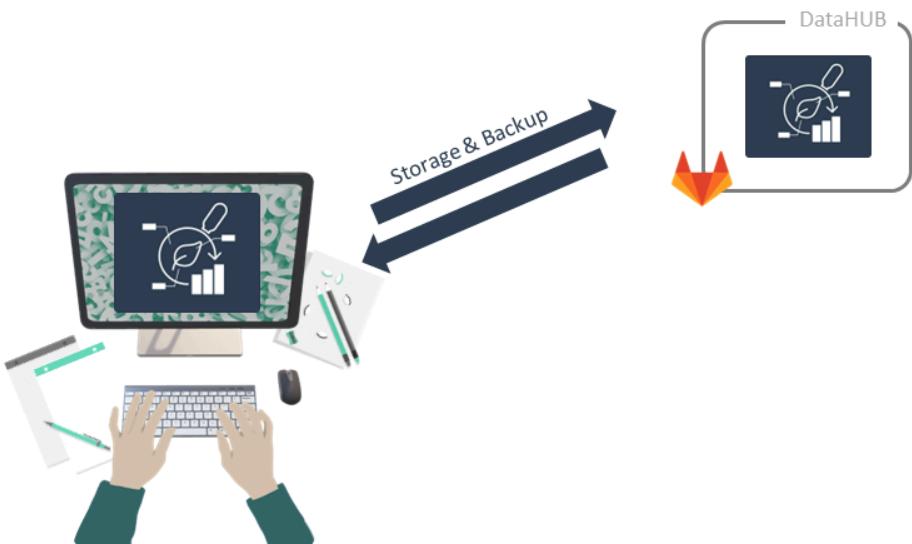


Annotated Research Context (ARC)

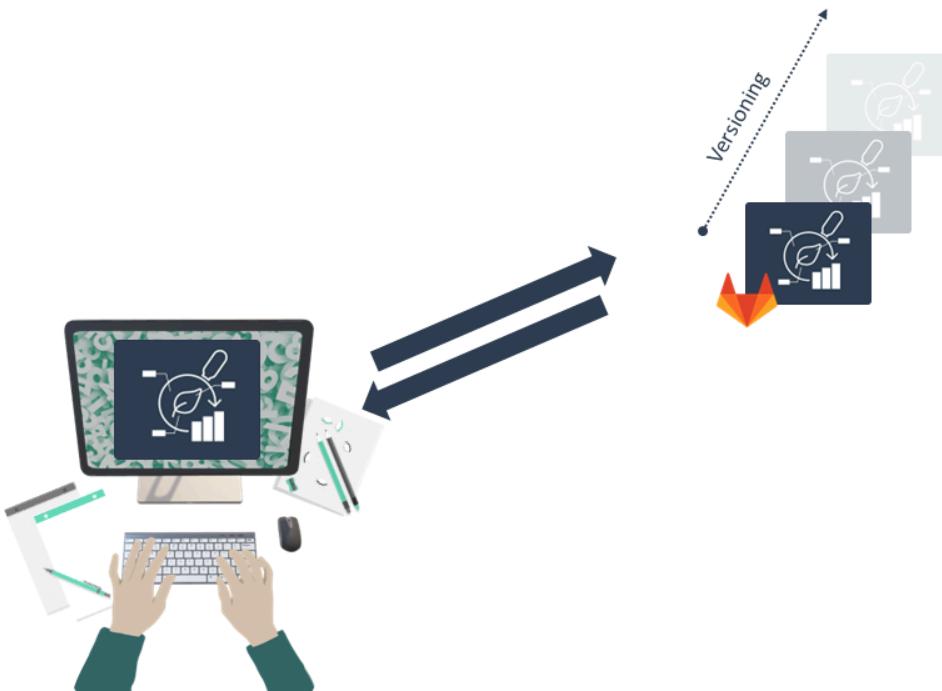


Your entire investigation in a single unified bag

You can store your ARC in the DataHUB



ARCs are versioned



You can invite collaborators



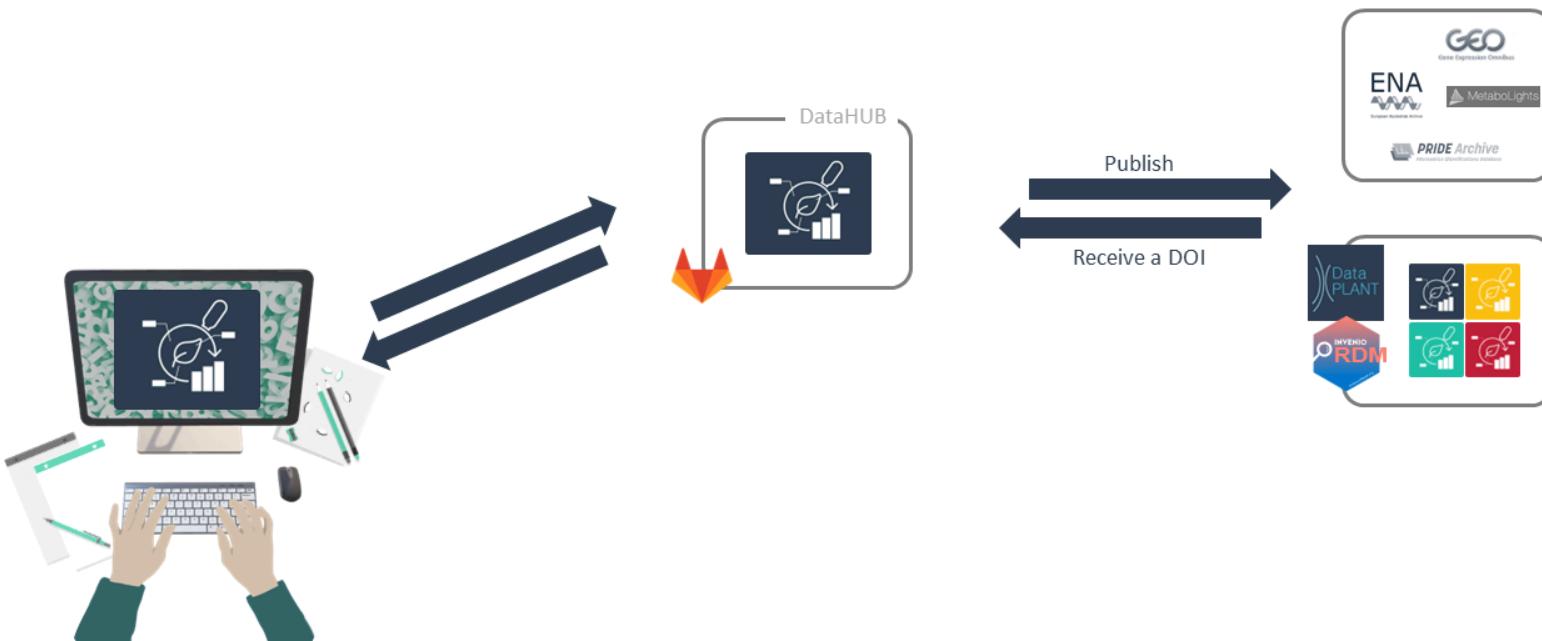
Collaborate and contribute



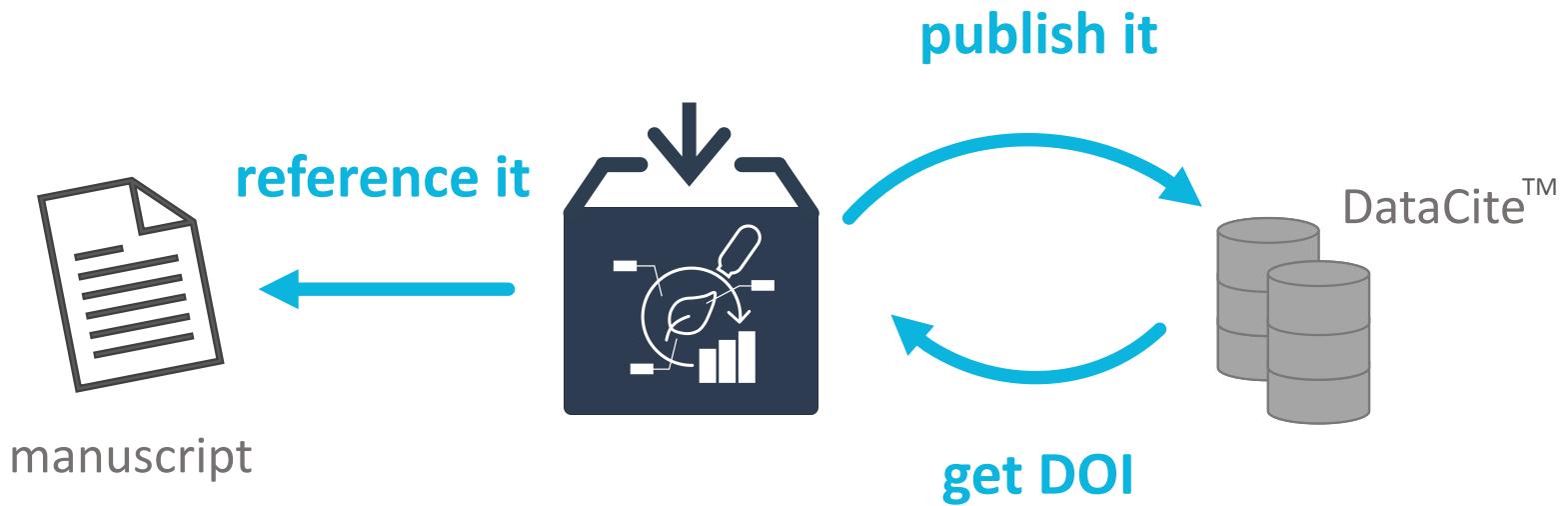
Reuse data in ARCs



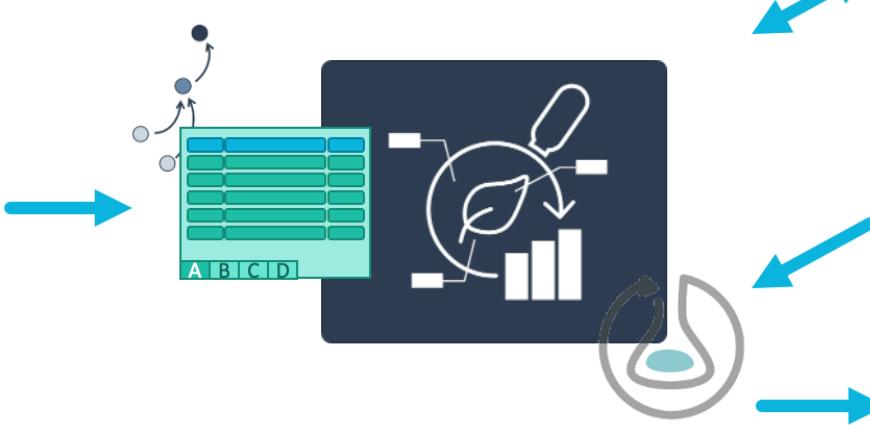
Publish your ARC



Publish your ARC, get a DOI



ARC as single-entry point



specialized endpoints

ENA
European Nucleotide Archive

GEO
Gene Expression Omnibus

PRIDE Archive
Proteomics Identifications database

EBI: MetaboLights

BioImage Archive

dataset search

Google

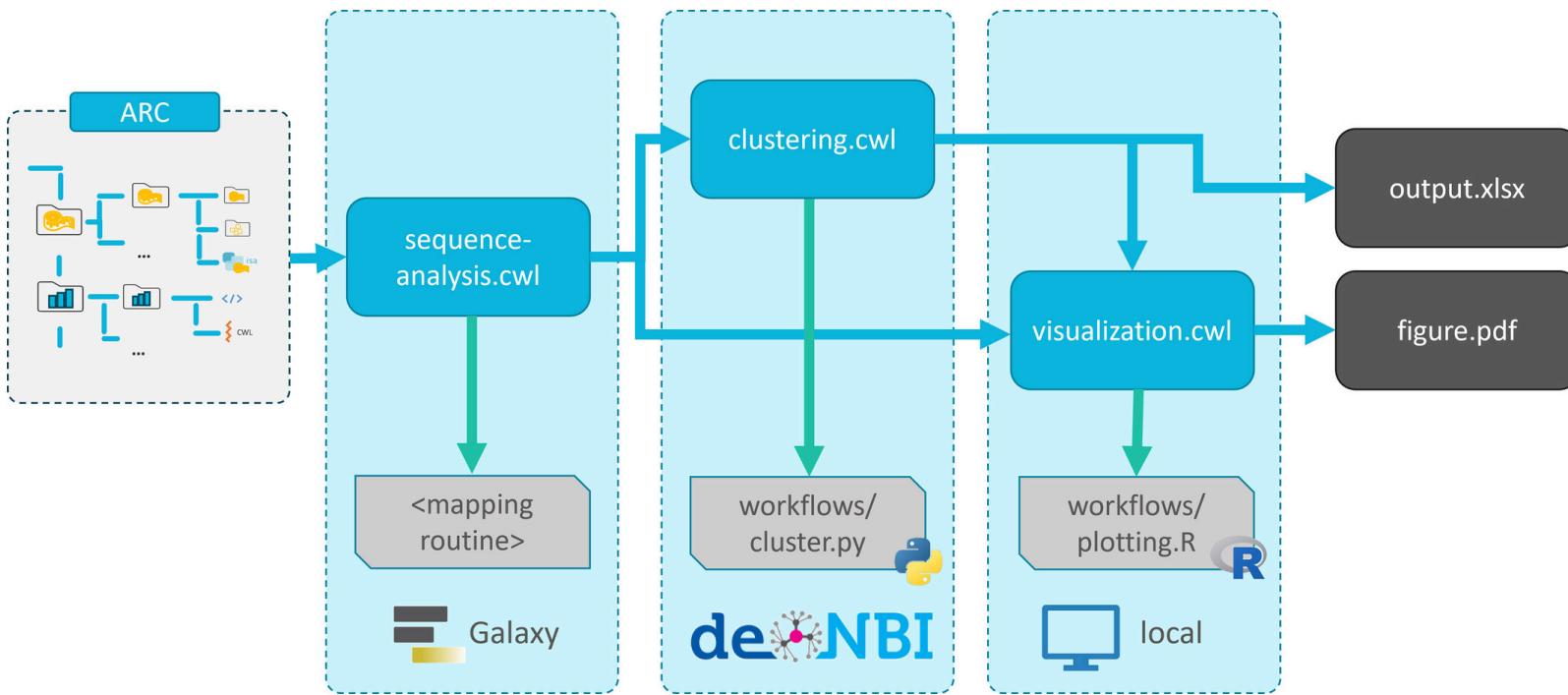
OpenAIRE

The Dataverse® Project

INVENIO

data publication

Data analysis and workflows



Galaxy integration: Extra value for plant research

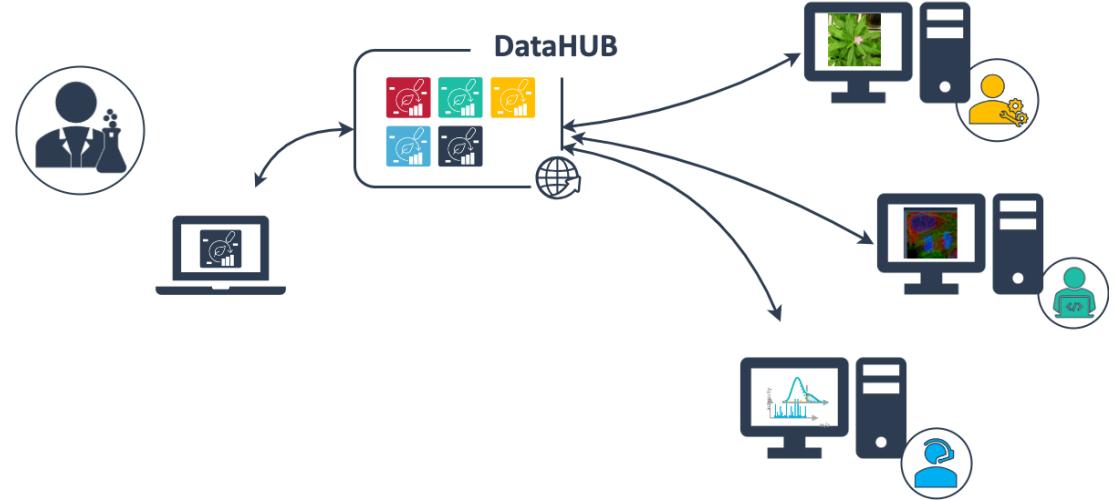


e.g. <https://plants.usegalaxy.eu>

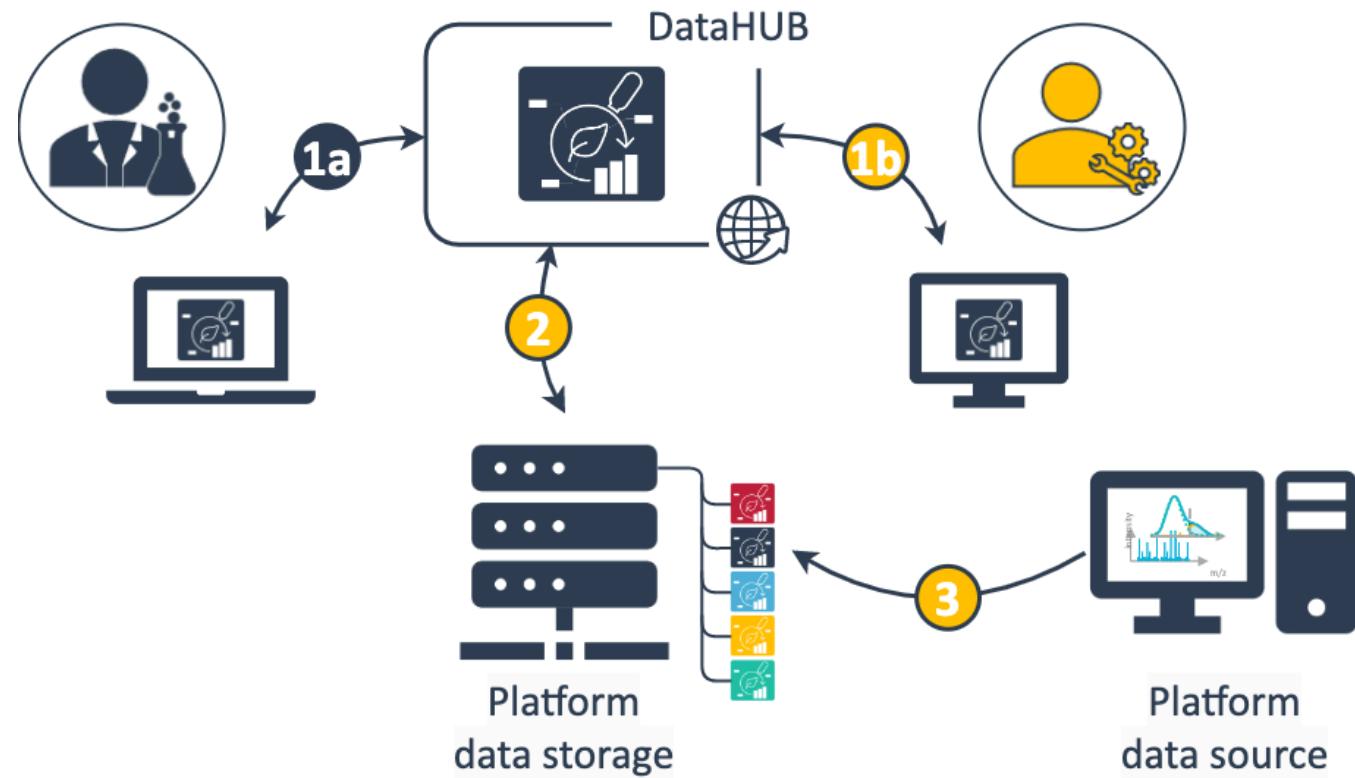
- Full ARC compatibility
- Automated metadata generation
- Specialized tools and workflows for ‘omics processing and analysis
- Public repository compatibility
- Galaxy teaching resource for data analysis

Enabling platforms

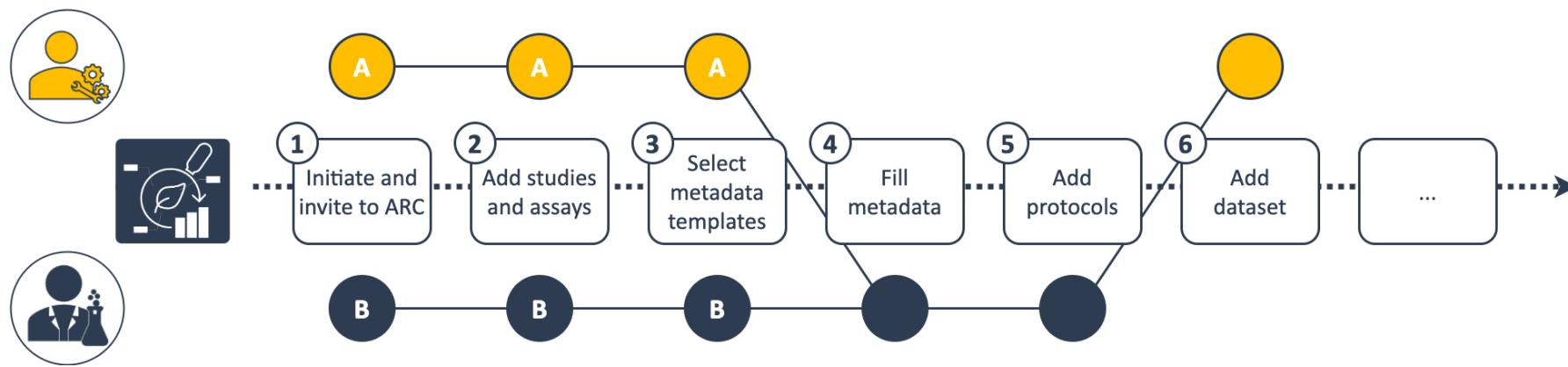
- Streamlined exchange of (meta)data
- Communication and project management



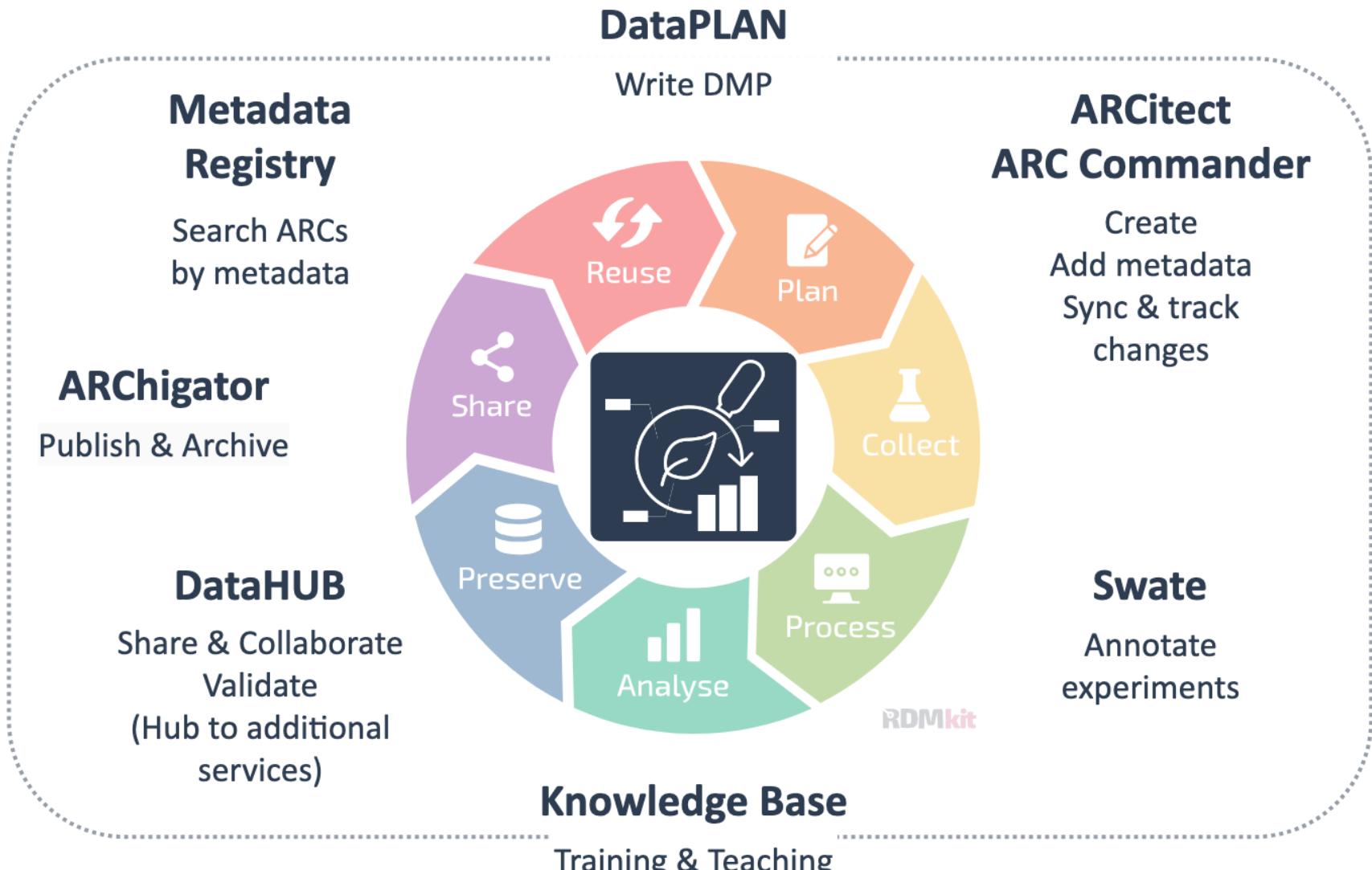
Streamlined data exchange



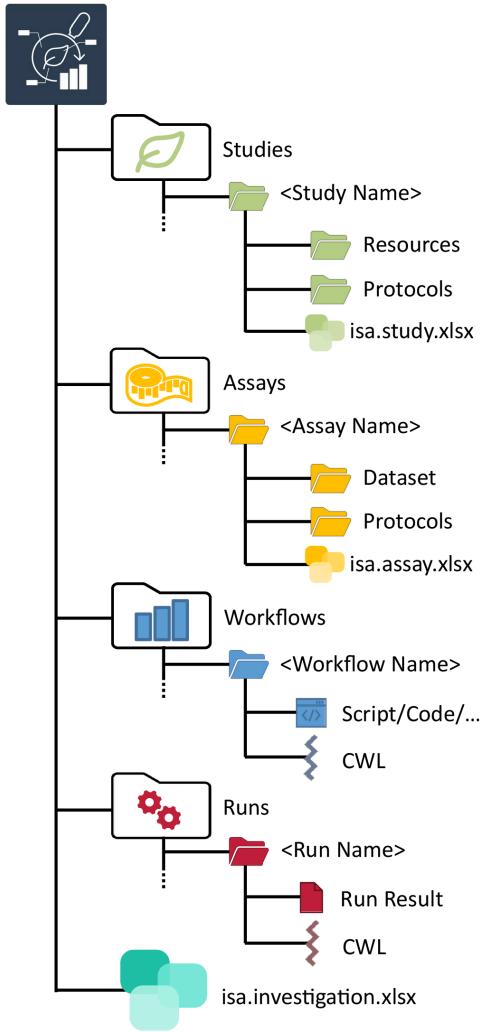
Meet your collaborators in an ARC



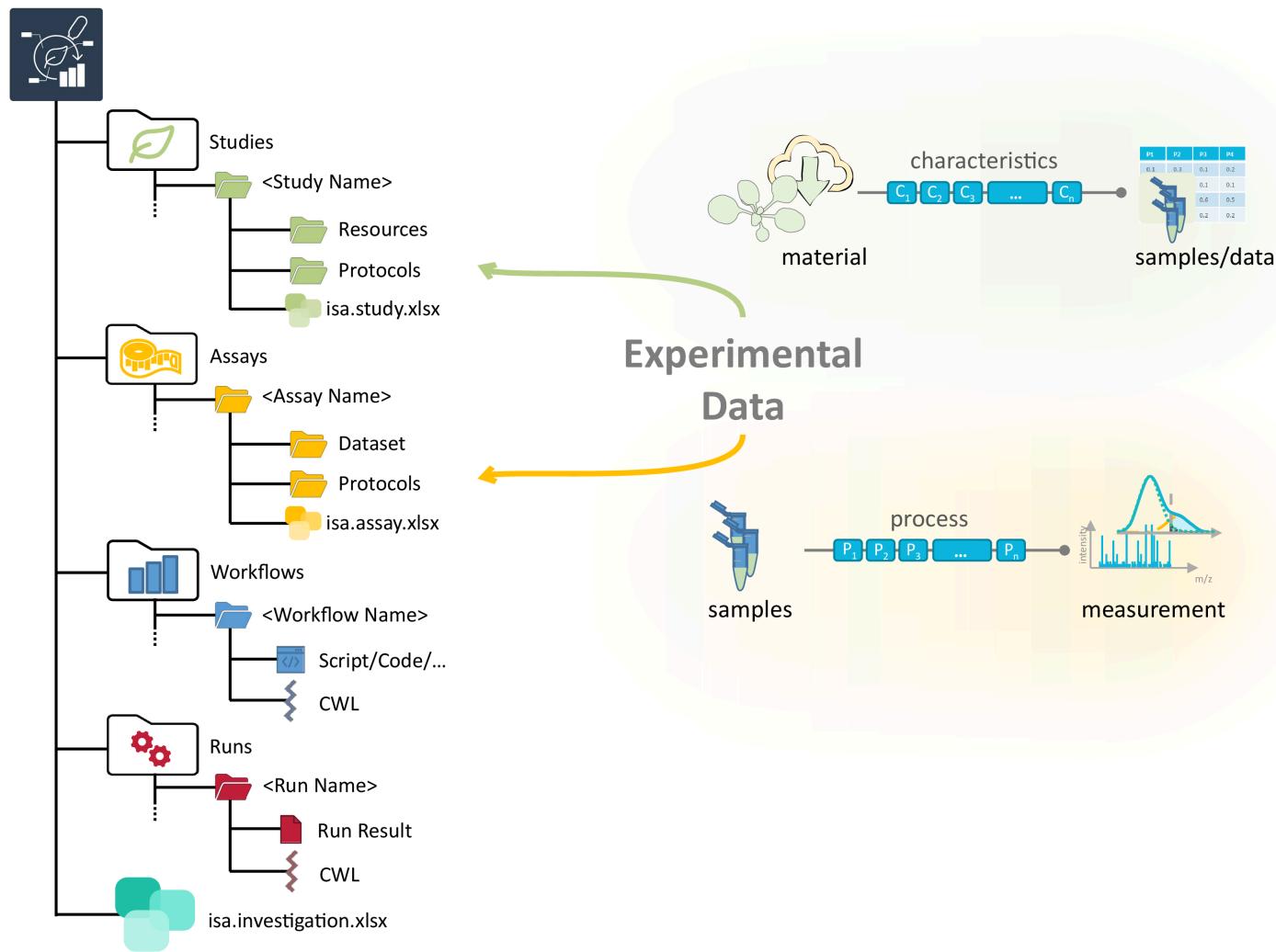
The ARC ecosystem



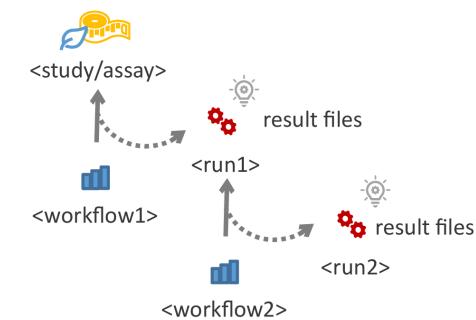
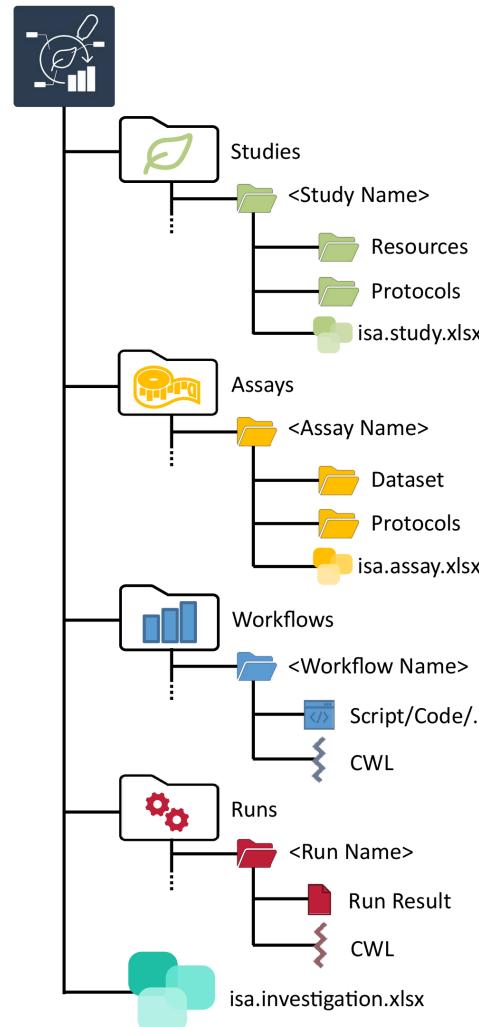
What does an ARC look like?



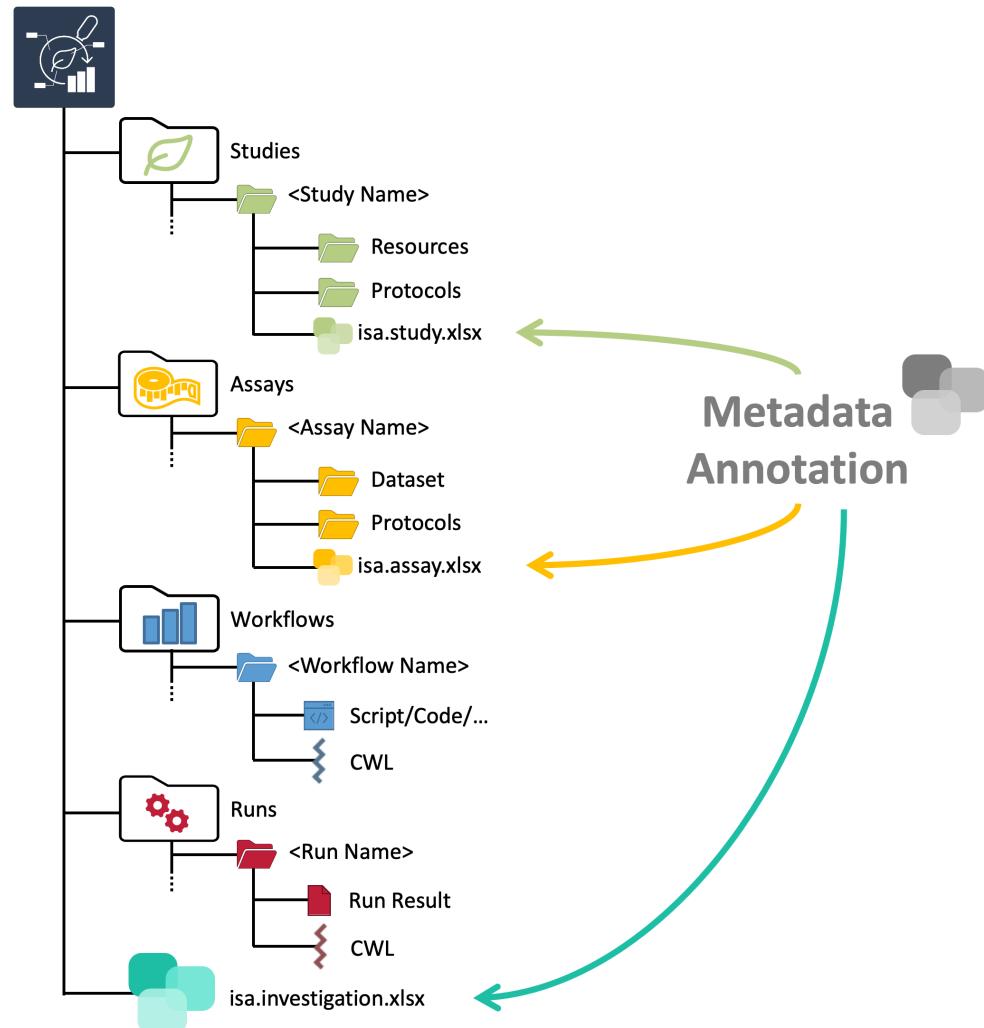
ARCs store experimental data



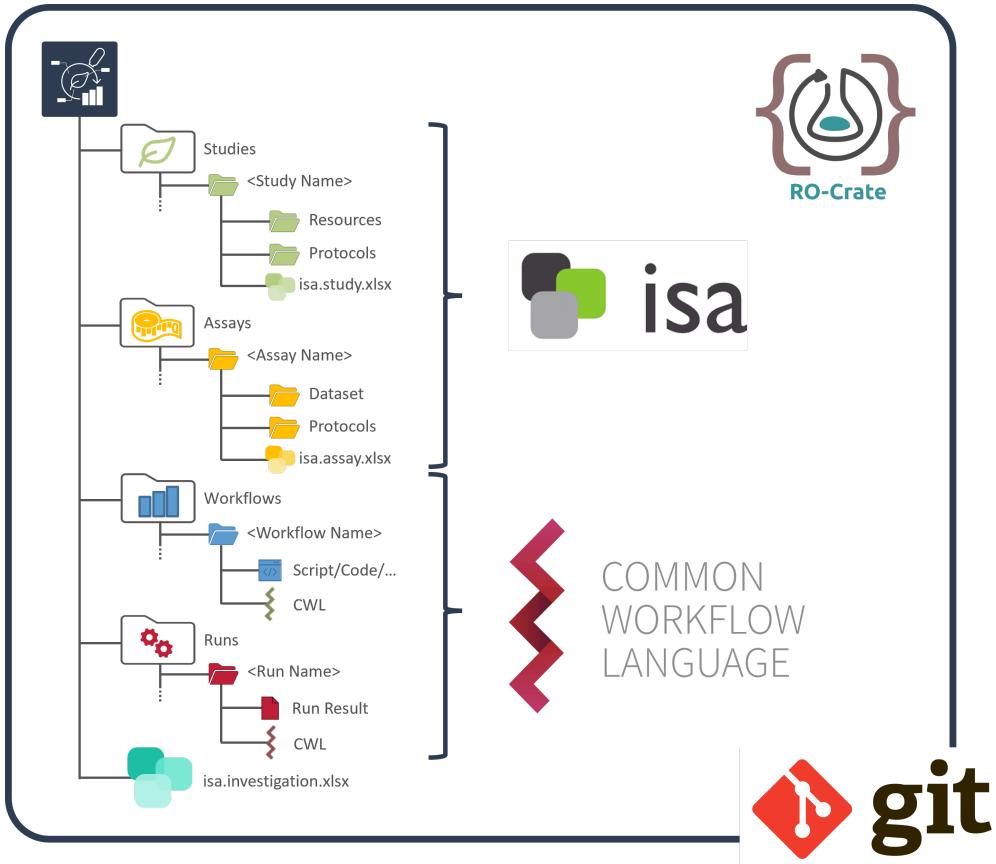
Computations can be run inside ARCs



ARCs come with comprehensive metadata



ARC builds on standards



- RO-Crate: standardized exchange
- ISA: structured, machine-readable metadata
- CWL: reproducible, re-usable data analysis
- Git: version control

ARCitect Hands-on

ARCitect installation

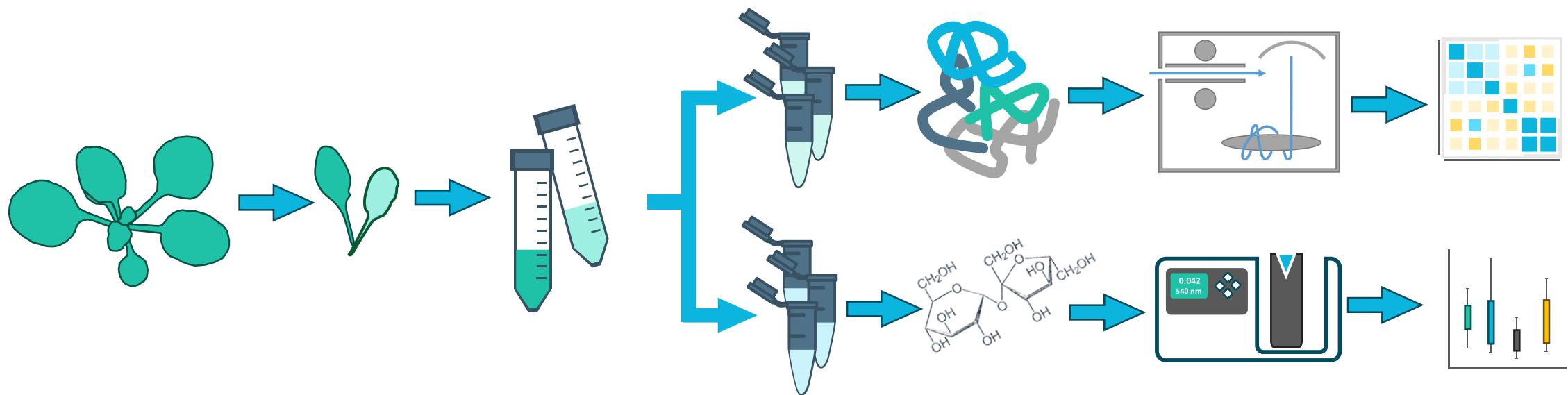
Please install version **v0.0.48** (or later) of the ARCitect:

<https://github.com/nfdi4plants/ARCitect/releases/latest>

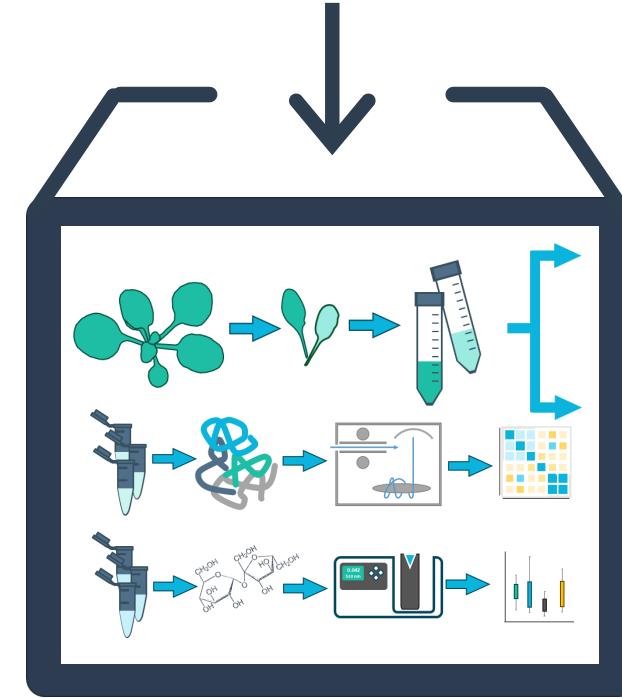
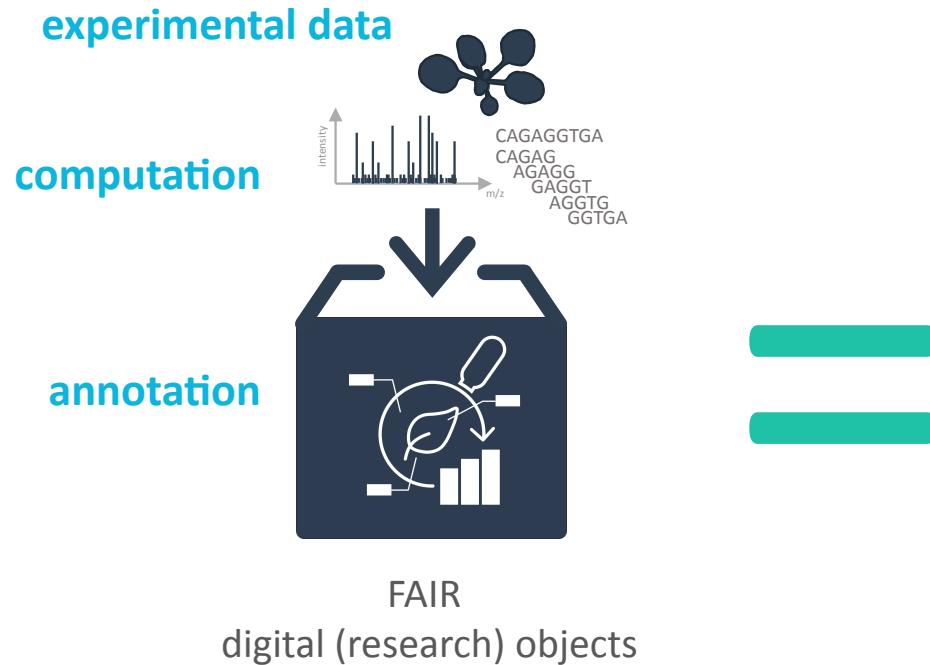
Download the demo data

<https://uni-duesseldorf.sciebo.de/s/C7ms3QA6q7OZnU2>

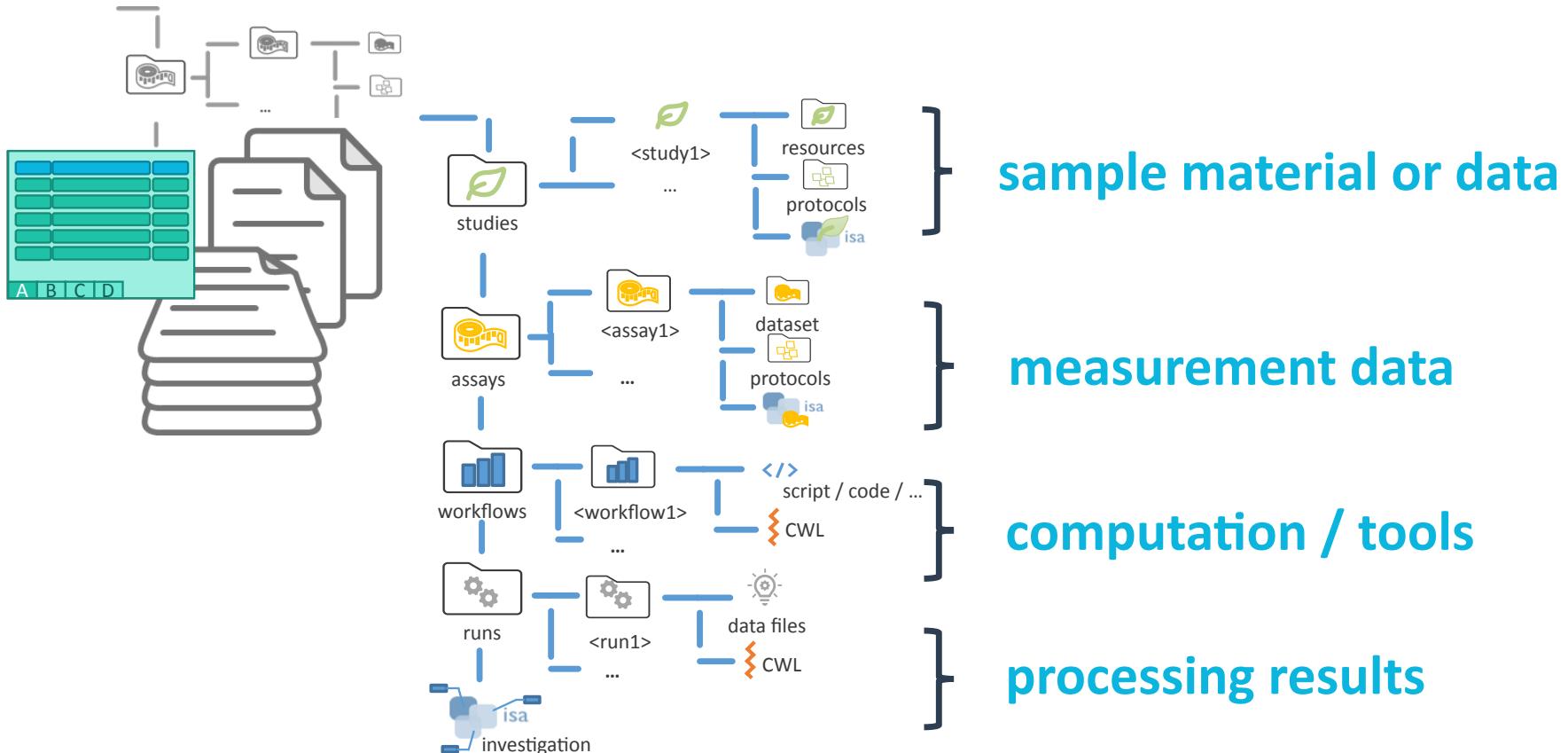
A small prototypic project



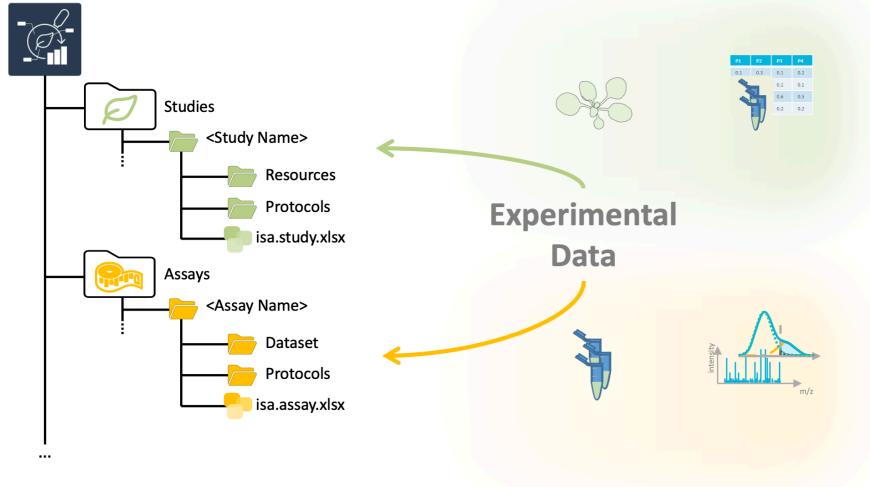
ARC: Annotated research context



The ARC scaffold structure



Sort Demo data in an ARC

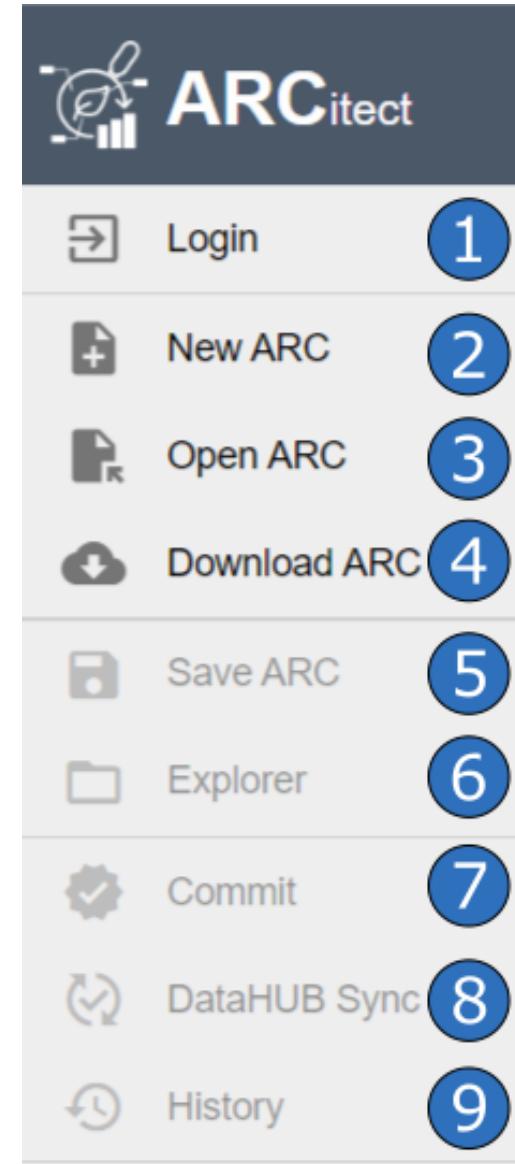


metabolomics_data
150112_56.D
150112_62.D
150112_66.D
150115_12.D
150115_14.D
150115_16.D
gcms_samplelist.tsv
method_gcms.txt
sample_submission_gcms.csv
methods
Illumina_libraries.txt
metabolite_extraction.txt
plant_material.txt
RNA_extraction.txt
rnaseq_data
DB_097_CAGATC_L001_R1_001.fastq.gz
DB_099_CTTGTA_L001_R1_001.fastq.gz
DB_103_AGTCAA_L001_R1_001.fastq.gz
DB_161_GTCCGC_L001_R1_001.fastq.gz
DB_163_GTGAAA_L001_R1_001.fastq.gz
DB_165_GTGAAA_L002_R1_001.fastq.gz
NGS_SampleSheet.xlsx

Initiate the ARC folder structure

1. Open ARCitect
2. Create a **New ARC** (2)
3. Select a location and name it

TalinumPhotosynthesis



Your ARC's name

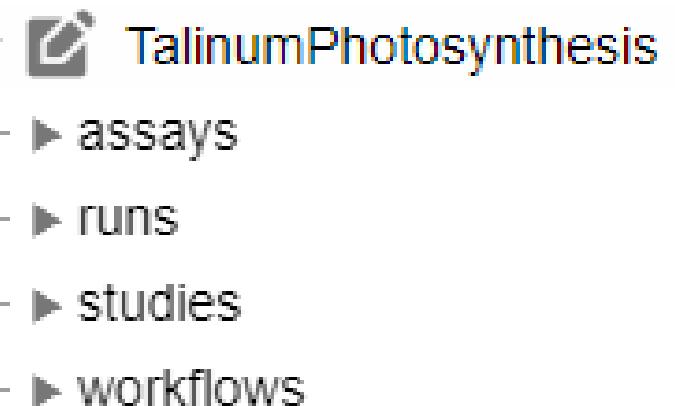
💡 By default, your ARC's name will be used

- 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 description to your investigation

C:/Users/Sabrina/Desktop/Workshops ARCs
/TalinumPhotosynthesis

TalinumPhotosynthesis

- assays
- runs
- studies
- workflows
-  .gitignore

1.34 KB

Identifier

Title

Description

This is a very interesting investigation about life and photosynthesis

Add contributors

- you could also add the contacts directly via ORCID

Contacts

Your First Name Your Last Name

Your ORCID

6/10 ▾

First Name

Last Name

Your First Name

Your Last Name

Mid Initials

ORCID

Your ORCID

Search

Affiliation

Address

Your Affiliation

Email

Phone

Fax

yourEmailAdress@uni.de

Roles

1.

Author



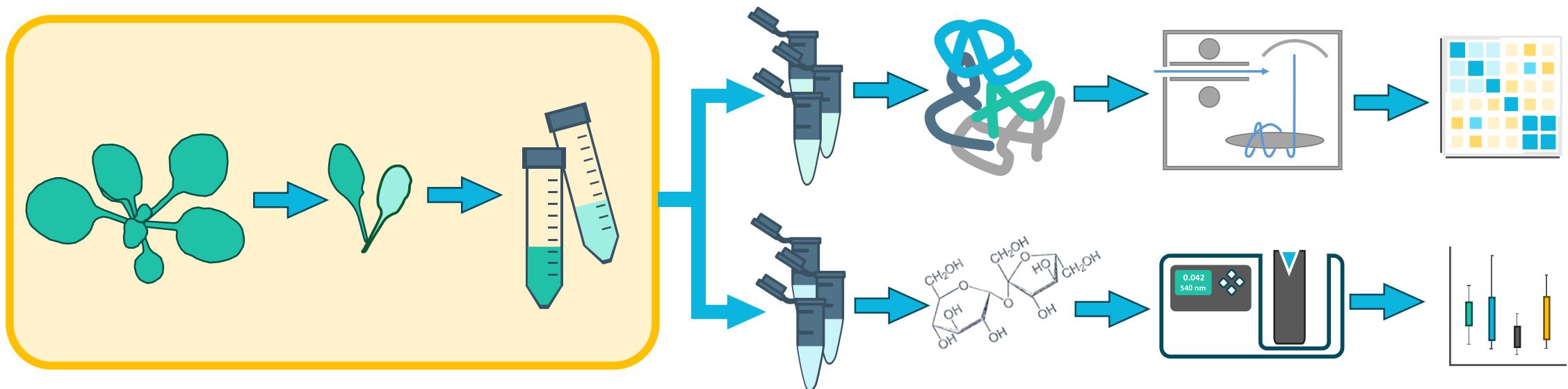
NCIT

NCIT:C42781

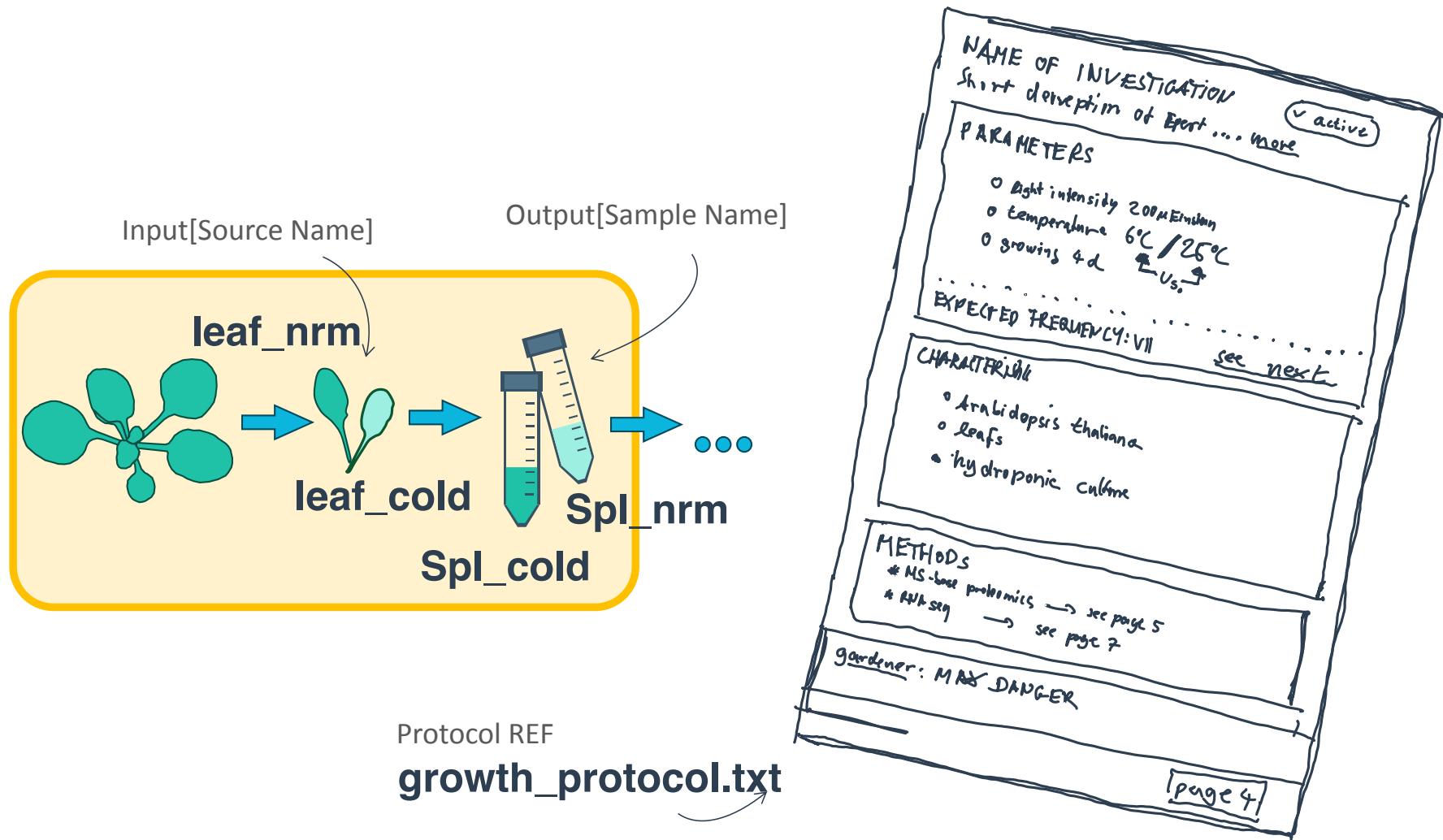


Delete

Divide and conquer for reproducibility



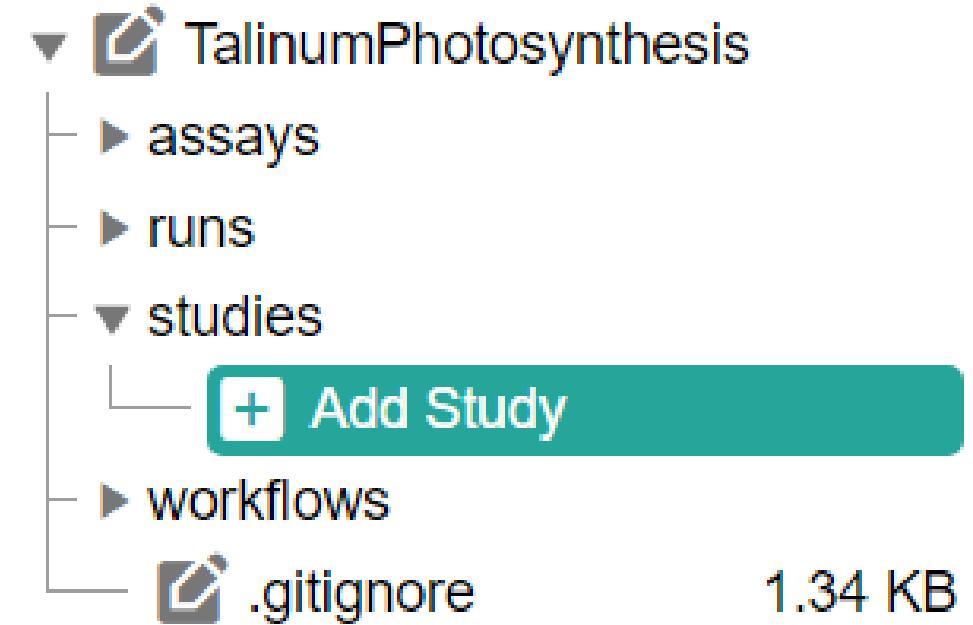
Identifying the 'study' part



Add a study

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

Use **talinum_drought** as an identifier



Study panel

In the study panel you can add

- general metadata,
- people, and
- publications
- data process information

Identifier
talinum_drought

Description

Contacts

Publications

Submission Date
tt.mm.jjjj --:--

Public ReleaseDate
tt.mm.jjjj --:--

Study Design Descriptors

Let's annotate the plant samples

1. Check out the lab notes

```
studies/talinum_drought/protocols/plant_material.txt
```

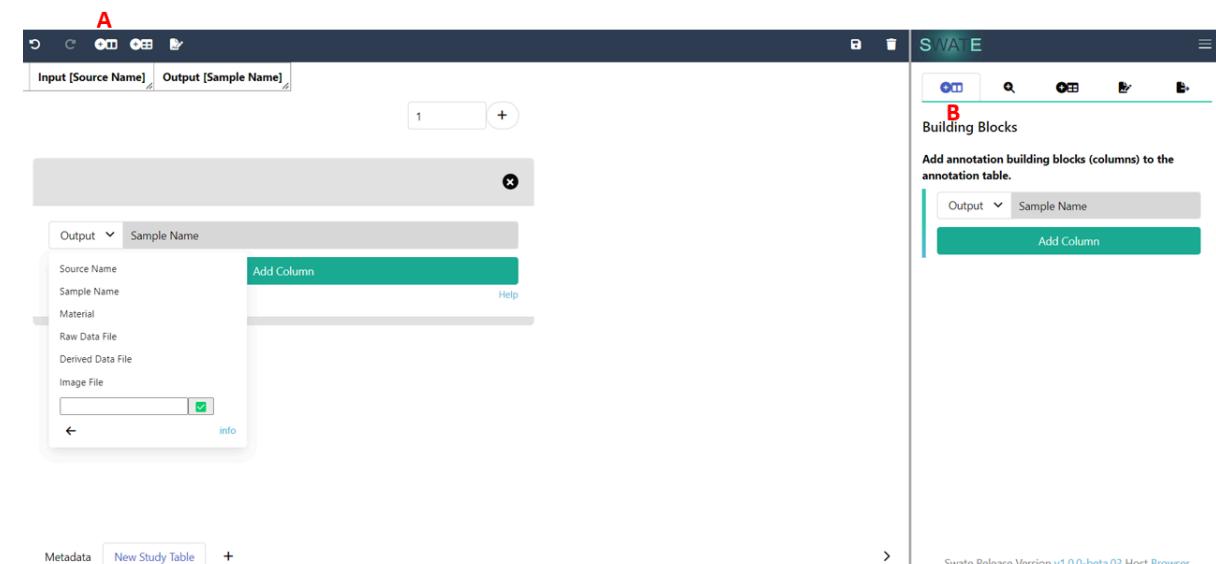
2. Select the study talinum_drought

3. Add a new table sheet at the bottom

Create an annotation table

1. Create a annotation table by adding **Building blocks** via the widget (A) or the sidebar (B)
2. Add an *Input* (Source Name) and *Output* (Sample Name) column

 Each table can contain only one *Input* and one *Output* column



A table-based organization schema

Input[Source Name]		Output[Sample Name]
leaf_nrm		spl_nrm
leaf_cold		spl_cold
A	B	C
D		

Fill out source name and sample name

Transfer the sample ids from the protocol.

1. Invent names for **Source Name** (we do not have this information)
2. Use the sample names from the protocol (DB_*) as **Sample Name**

Add protocols

You can either

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

Create or Import Protocol

Protocol Name



NEW PROTOCOL



IMPORT PROTOCOL

CANCEL

Link the protocol to the isa table

1. In the *Building Blocks* tab, select *More* -> *Protocol REF*.
2. Click  *Add Column*.
3. Add the name of the protocol file (`plant_material.txt`) to the *Protocol REF* column.

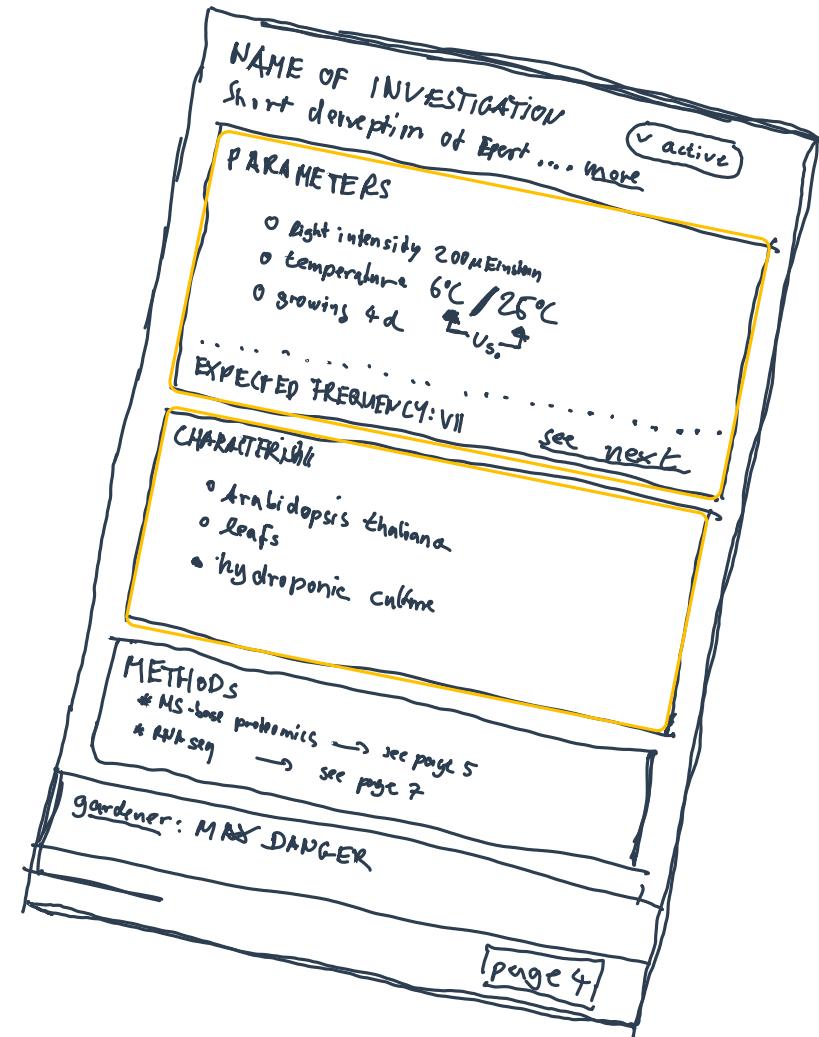
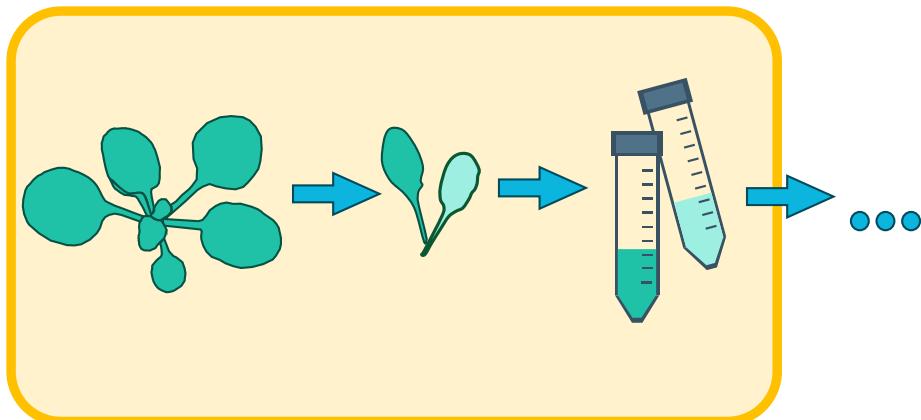
Referencing a protocol

This allows you to reference the free-text, human-readable protocol.

Input[Source Name]	Protocol REF	Output[Sample Name]
leaf_nrm	growth_protocol.txt	spl_nrm
leaf_cold	growth_protocol.txt	spl_cold
A	B	C
D		

- 💡 It is recommended that the protocol is in an open format (.md|.txt|.docx|...)
- 💡 But everything is possible also an URI to an electronic lab notebook

Parameterizing the 'study'



Finding the right metadata vocabulary

Parameters []

- Light intensity 200 µEinstein
- Temperature 6°C / 25°C
- Growing 4d

Characteristics []

- *Arabidopsis thaliana*
- Leaf
- Hydroponic culture
- Columbia

OLS: Finding the right metadata vocabulary

Temperature Dependence [Temperature:Dependence_Annotation](#)

http://purl.uniprot.org/core/Temperature_Dependence_Annotation

Indicates the optimum temperature for enzyme activity and/or the variation of enzyme activity with temperature variation; the thermostability/thermolability of the enzyme is also mentioned when it is known.

Ontology: [UNIPROT RDFS](#)

temperature [AFO:/result#AFR_0001584](#)

http://purl.allotrope.org/ontologies/result#AFR_0001584

A temperature (datum) is a quantity facet that quantifies some temperature. [Allotrope]

Ontology: [AFO](#)

temperature [FBcv:0000466](#)

http://purl.obolibrary.org/obo/FBcv_0000466

Mutation caused by exposure to a temperature that is higher or lower than 25 degrees Celsius.

Ontology: [FBCV](#)

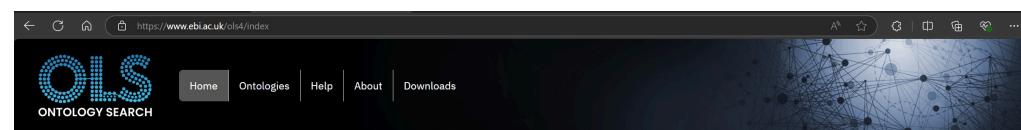
temperature [PATO:0000146](#)

http://purl.obolibrary.org/obo/PATO_0000146

A physical quality of the thermal energy of a system.

Ontology: [PATO](#)

Also appears in: [NGBO](#) [HTN](#) [CAO](#) [ZP](#) [AGRO](#) [OMIABIS](#) [OBIB](#) [MONDO](#) [TXPO](#) [MCO](#) +



Welcome to the EMBL-EBI Ontology Lookup Service

temperature

Exact match Include obsolete terms Include imported terms

Examples: diabetes, GO:0098743

Looking for a particular ontology?

About OLS
The Ontology Lookup Service (OLS) is a repository for biomedical ontologies that aims to provide a single point of access to the latest ontology versions. You can browse the ontologies through the website as well as programmatically via the OLS API. OLS is developed and maintained by the Samples, Phenotypes and Ontologies Team (SPOT) at EMBL-EBI.

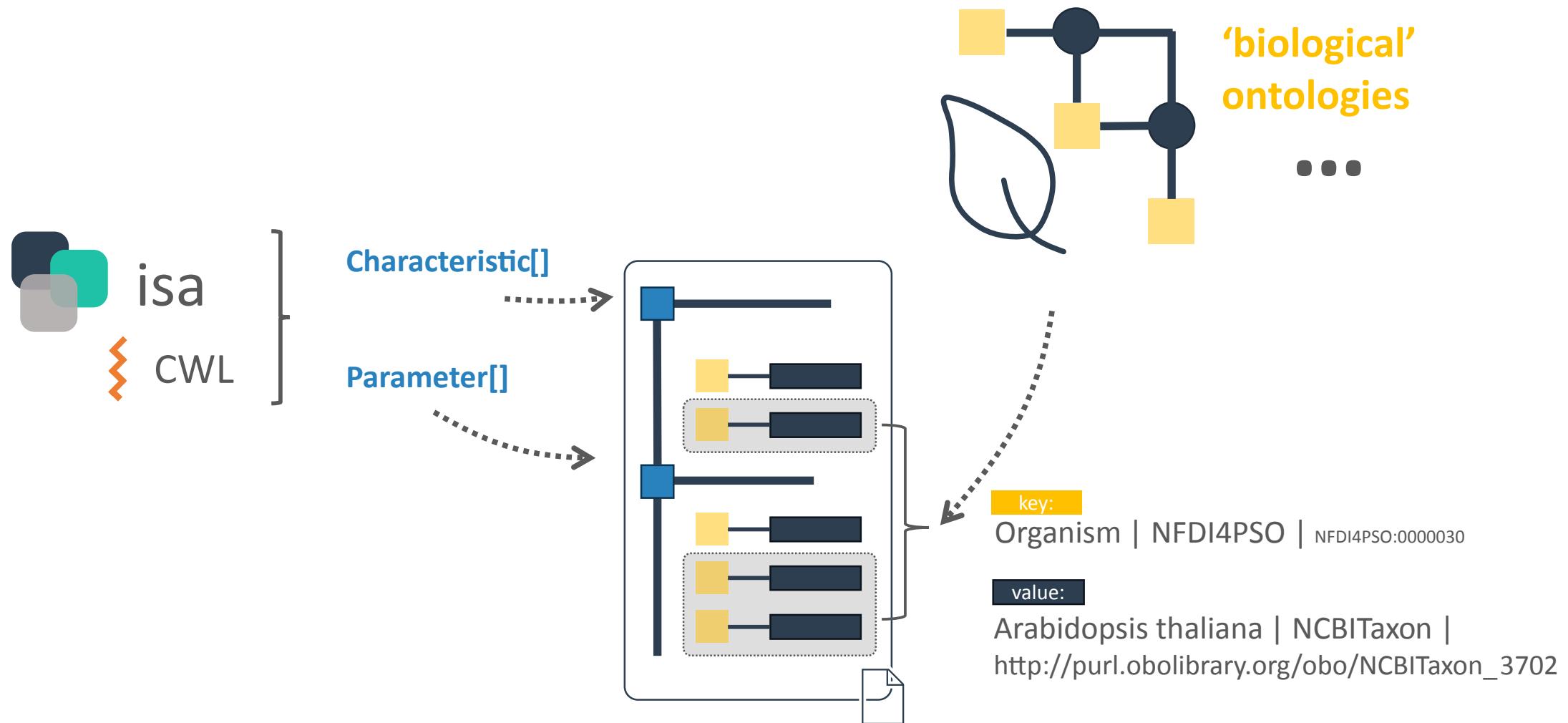
Related Tools
In addition to OLS the SPOT team also provides the OxO and ZOOMA services. OxO provides cross-ontology mappings between terms from different ontologies. ZOOMA is a service to assist in mapping data to ontologies in OLS.

Report an Issue
For feedback, enquiries or suggestion about OLS or to request a new ontology please use our GitHub issue tracker. For announcements relating to OLS, such as new releases and new features sign up to the OLS announce mailing list.

FOLLOW US

EMBL-EBI 2023 Licensing

Finding the metadata vocabulary and descriptors



Finding the metadata vocabulary and descriptors

Parameters []

- 
- 
- 
-  Light intensity 200 μ Einstein
-  Temperature 6°C / 25°C
-  Growing 4d

Characteristics []

- 
- 
- 
-  *Arabidopsis thaliana*
-  Leaf
-  Hydroponic culture
-  Columbia

Finding the metadata vocabulary and descriptors

Parameters []

-  Light intensity
 -  200 µEinstein
-  Temperature
 -  6°C / 25°C
-  Growth time
 -  4d

Characteristics []

-  Organism
 -  Arabidopsis thaliana
-  Tissue
 -  Leaf
-  Growth medium
 -  Hydroponic culture
-  Ecotype
 -  Columbia

Annotation Building Block types

- Input (e.g. Source Name, Sample Name)
- Protocol columns
- Characteristic // Parameter // Factor //
- Component
- Output (e.g. Sample Name, Raw Data File, Derived Data File)

The screenshot shows a software interface for managing annotation building blocks. At the top, there's a toolbar with various icons. Below it is a header bar labeled "Widgets". The main area contains a table with six rows of data:

Input [Source Name]	Characteristic [organism]	Factor [watering exposure]	Output [Sample Name]
DB_097	Talinum fruticosum	✓ 12 days drought	CAM_01
DB_099	Talinum fruticosum	✓ 12 days drought	CAM_02
DB_103	Talinum fruticosum	✓ 12 days drought	CAM_03
DB_161	Talinum fruticosum	✓ 12 days drought + 2 days rewetared	reC3_01
DB_163	Talinum fruticosum	✓ 12 days drought + 2 days rewetared	reC3_02
DB_165	Talinum fruticosum	✓ 12 days drought + 2 days rewetared	reC3_03

Annotations are overlaid on the table:

- "Factor" is highlighted in blue over the "Factor" column.
- "Input" is highlighted in blue over the first column.
- "Characteristic" is highlighted in blue over the second column.
- "Output" is highlighted in blue over the fourth column.

To the right of the table is a "New Parameter" dialog box with tabs for "Parameter", "Factor", "Characteristic", "Component", and "More". The "Parameter" tab is selected. A "Sidebar" button is located at the bottom right of the dialog.

Let's take a detour on [Annotation Principles](#)

Add Characteristics

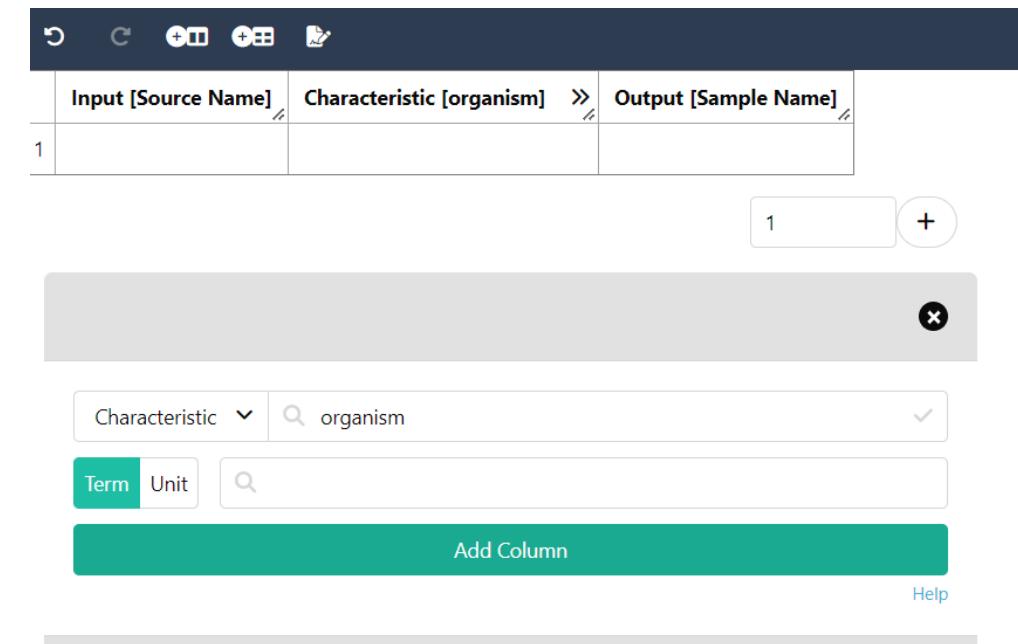
1. Select *Characteristic* from the drop-down menu

2. Enter **organism** in the search bar. This search looks for suitable *Terms* in our *Ontology* database.

3. Select the Term with the id **OBI:0100026** and,

4. Click **Add Column**

 This adds four columns to your table, one visible and **three** hidden.



Input [Source Name]	Characteristic [organism]	Output [Sample Name]
1	organism	

Characteristic

Term

Help

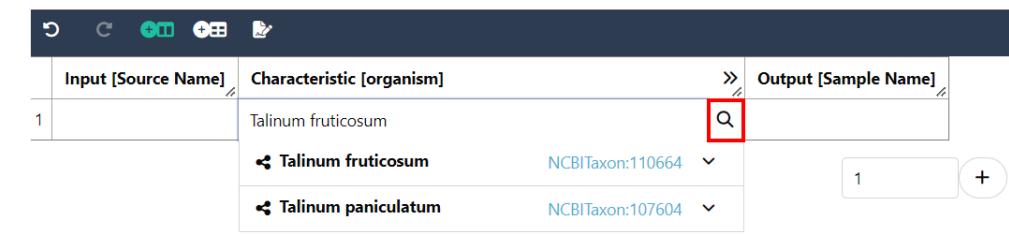
Insert ontology terms

1. Insert values by selecting any cell below

Characteristic [organism]

2. Use free text or use the magnifying glass to activate *Term* search

3. Write "Talinum fruticosum" and enable *Term* search
4. Select the hit



Add a Parameter building block with a unit

1. In the *Building Blocks* widget, select *Parameter*, search for `light intensity exposure` and select the term with id `PEC0:0007224`.
2. Check the box for *Unit* and search for `microeinsteins per square meter per second` in the adjacent search bar.
3. Select `U0:0000160`.
4. Click Add Column.

 This also adds four columns to your table, one visible and **three** hidden.

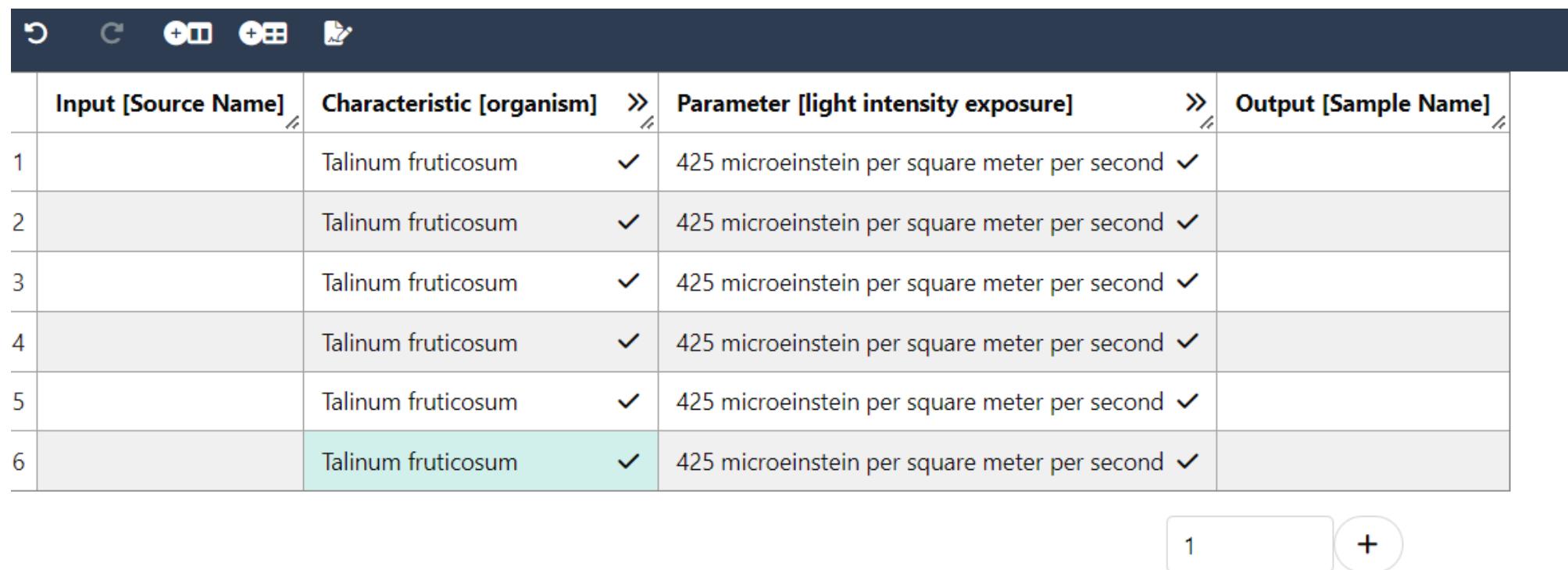
Insert unit-values

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 microeinstein per square meter per second

Your annotation table is growing

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



The screenshot shows a user interface for managing an annotation table. At the top, there is a dark header bar with five icons: a circular arrow, a 'C' for copy, a plus sign with a document icon, a plus sign with a grid icon, and a pencil icon. Below the header is a table with the following structure:

Input [Source Name]	Characteristic [organism] >>	Parameter [light intensity exposure] >>	Output [Sample Name]
1	Talinum fruticosum ✓	425 microeinsteins per square meter per second ✓	
2	Talinum fruticosum ✓	425 microeinsteins per square meter per second ✓	
3	Talinum fruticosum ✓	425 microeinsteins per square meter per second ✓	
4	Talinum fruticosum ✓	425 microeinsteins per square meter per second ✓	
5	Talinum fruticosum ✓	425 microeinsteins per square meter per second ✓	
6	Talinum fruticosum ✓	425 microeinsteins per square meter per second ✓	

Below the table, there is a small control panel with a '1' button and a '+' button.

Exercise

Try to add suitable *Building Blocks* for other pieces of metadata from the plant growth protocol (`studies/talinum_drought/protocols/plant_material.txt`).

Add a factor building block

1. In the *Building Blocks* widget, select *Factor*, search for `watering exposure` and select the term with id `PEC0:0007383`.
 2. Click `Add Column`.
 3. Add the drought treatment ("no water for 12 days", "re-water for 2 days") to the respective samples
-  There are different options to add the drought treatment.

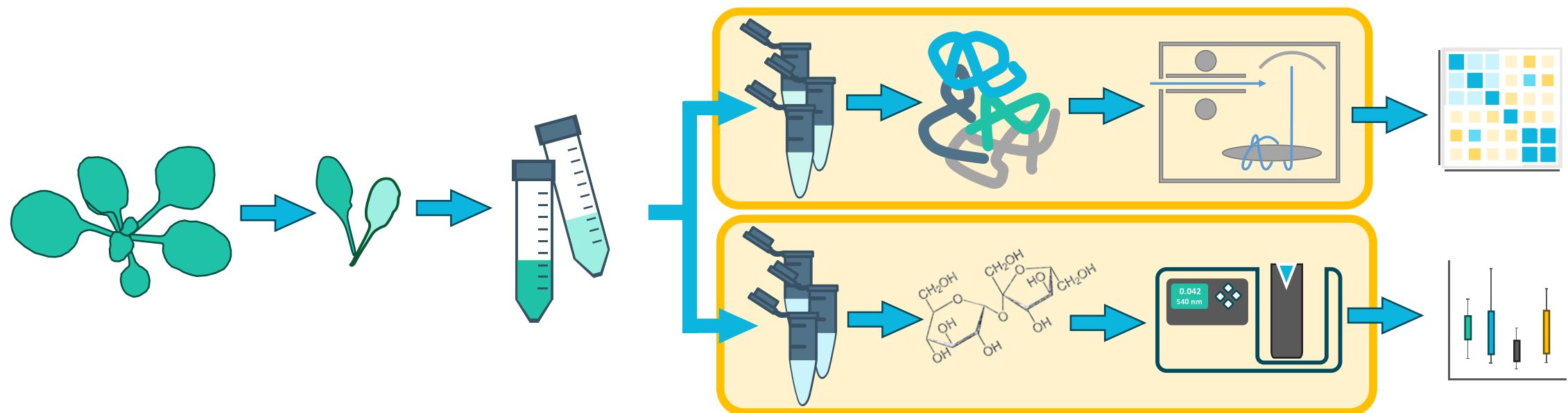
Showing ontology reference columns

Use double pointed quotation mark to un-hide hidden columns.

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

Characteristic [organism]	Unit	TSR (OBI:0100026)	TAN (OBI:0100026)
Talinum fruticosum	-	NCBITaxon	NCBITaxon:110664

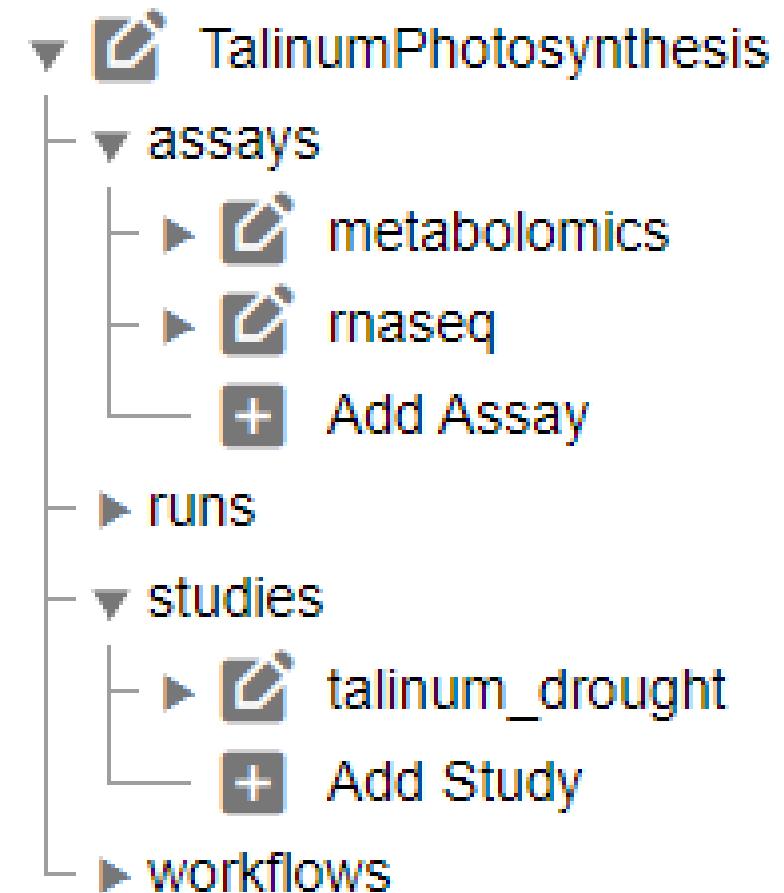
Identifying assays



Add an assay

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

Add two assays with **rnaseq** and **metabolomics** as an identifier



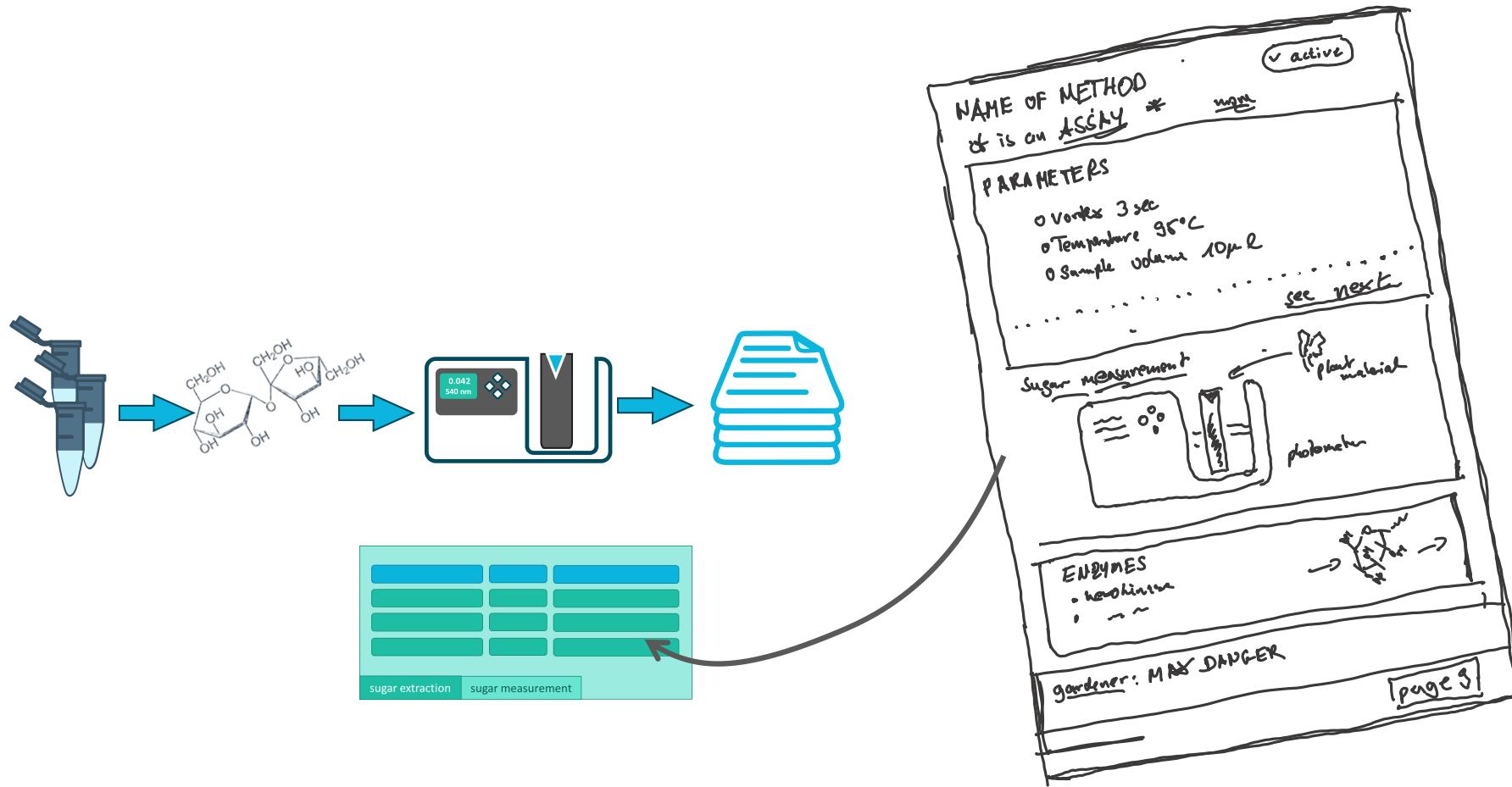
Add information about your assay

In the assay panel you can define the assay's

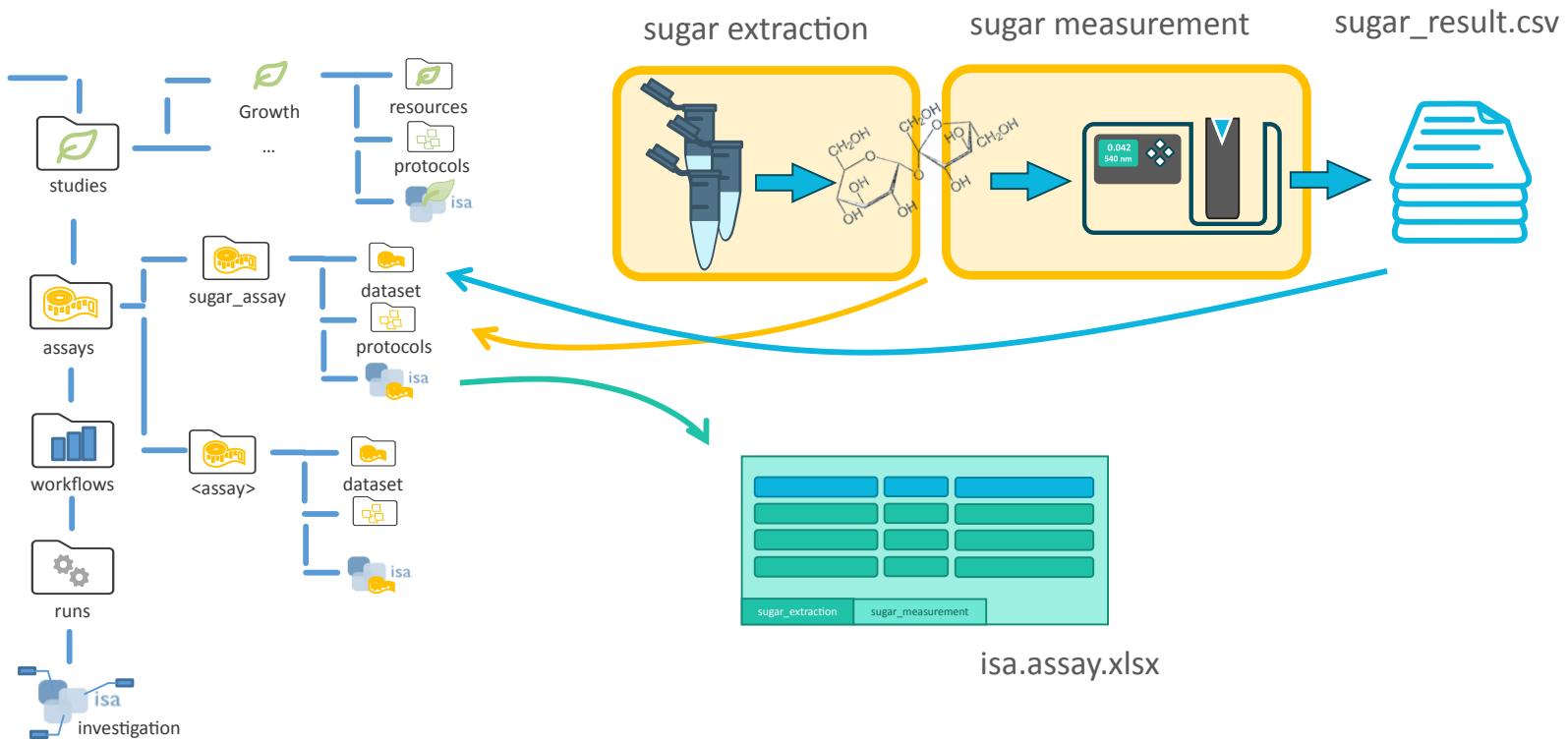
- measurement type
- technology type, and
- technology platform

Identifier		
rnaseq		
Measurement Type		
Term Name	TSR	TAN
<input type="text"/>	<input type="text"/>	<input type="text"/>
Technology Type		
Term Name	TSR	TAN
<input type="text"/>	<input type="text"/>	<input type="text"/>
Technology Platform		
Term Name	TSR	TAN
<input type="text"/>	<input type="text"/>	<input type="text"/>
Performers		
<input type="button" value="+"/>		
Comments		
<input type="button" value="+"/>		

Assay for sugar measurement



Separating different assay elements



Parametric description of the lab process

sugar extraction

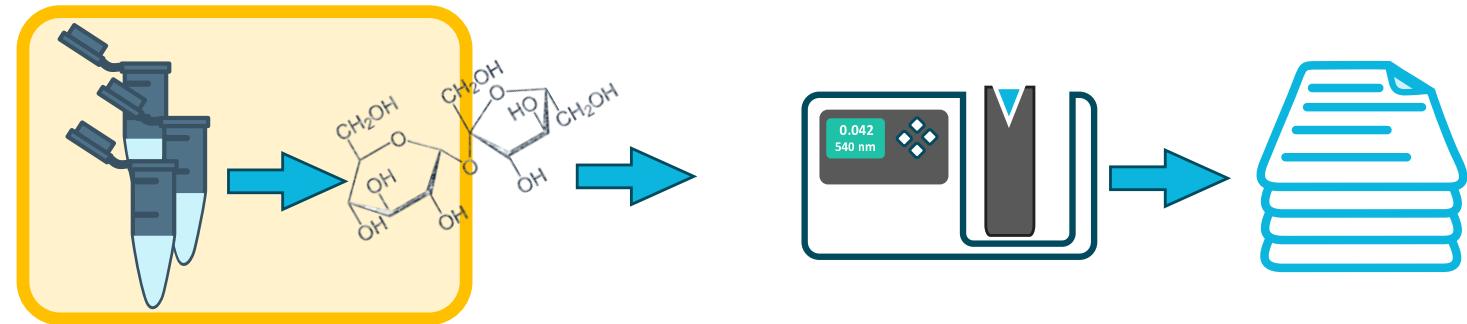
- Parameter []

- Temperature

- 95 °C

- Vortex Mixer

- 3 s



Parametric description of the lab process

- Parameter []

- technical replicate

- 1-3

- sample volume

- 10 µl

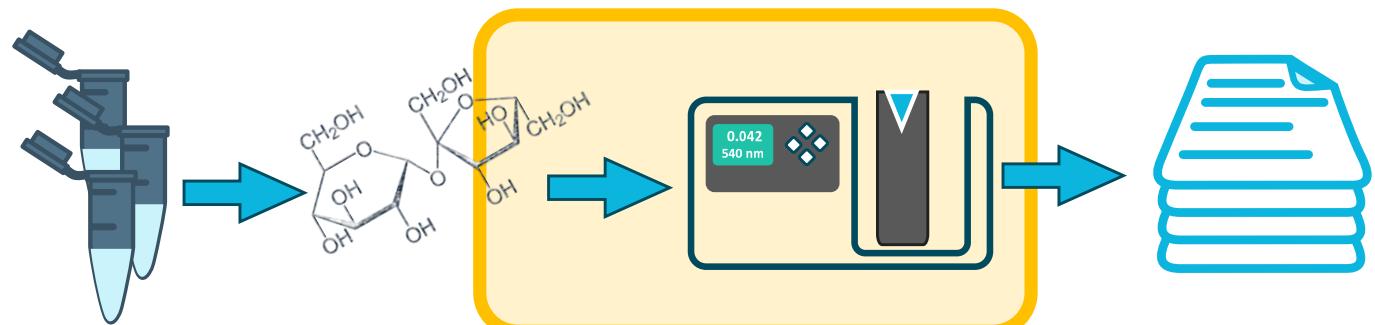
- Buffer

- 190 µl

- Cycle

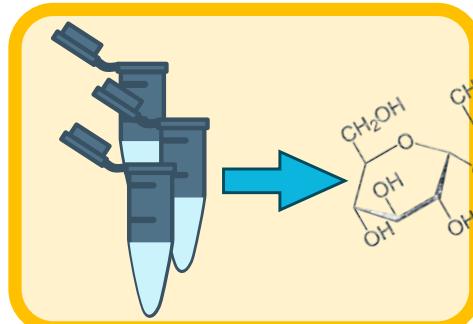
- 5

sugar measurement

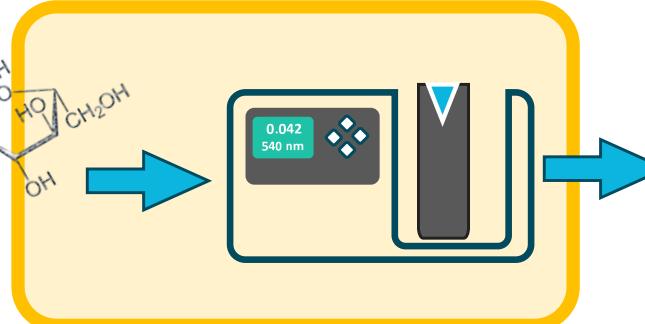


Isolating the lab processes in an assay

sugar extraction

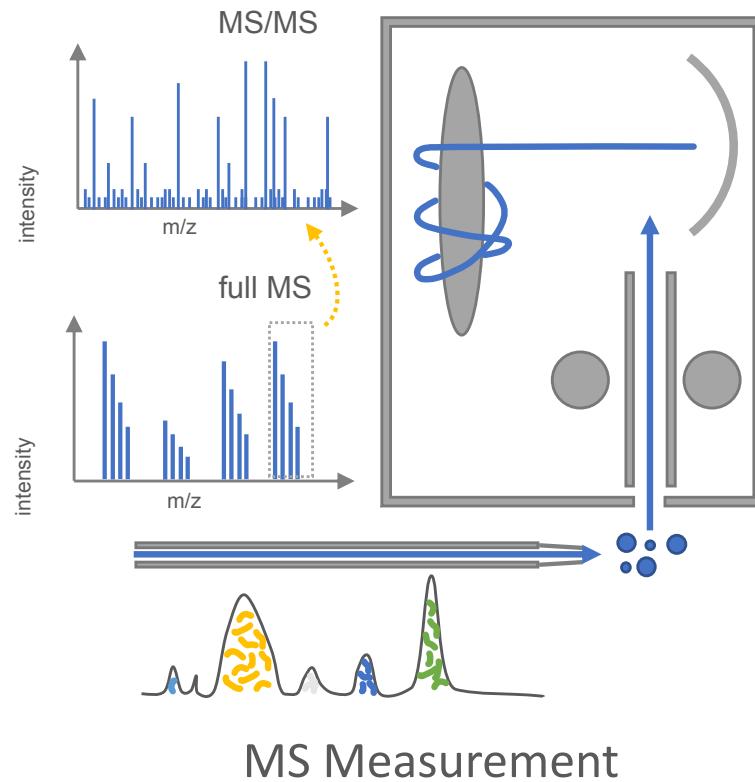


sugar measurement



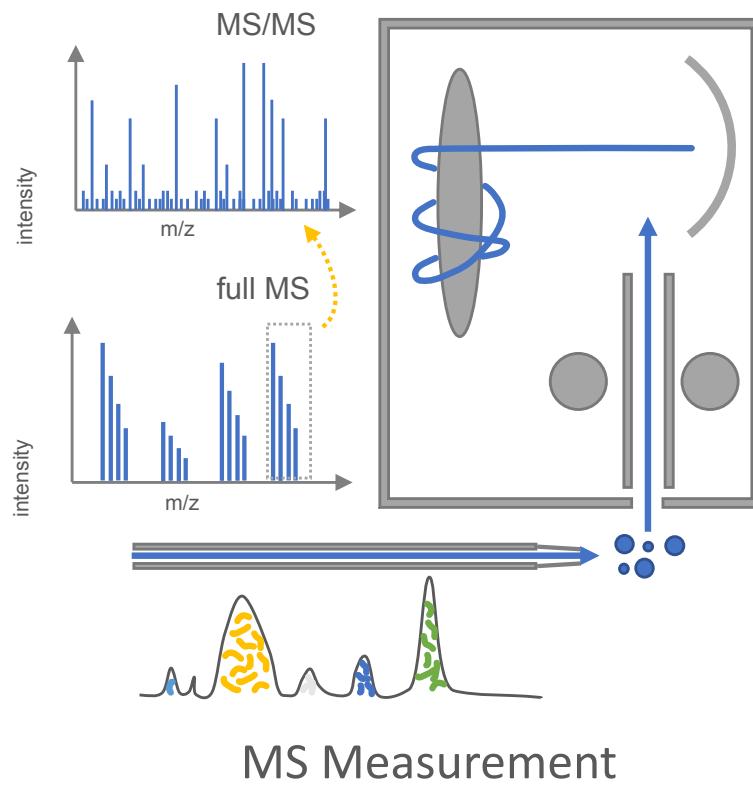
sugar_result.csv

Save time using standard methods and SOPs



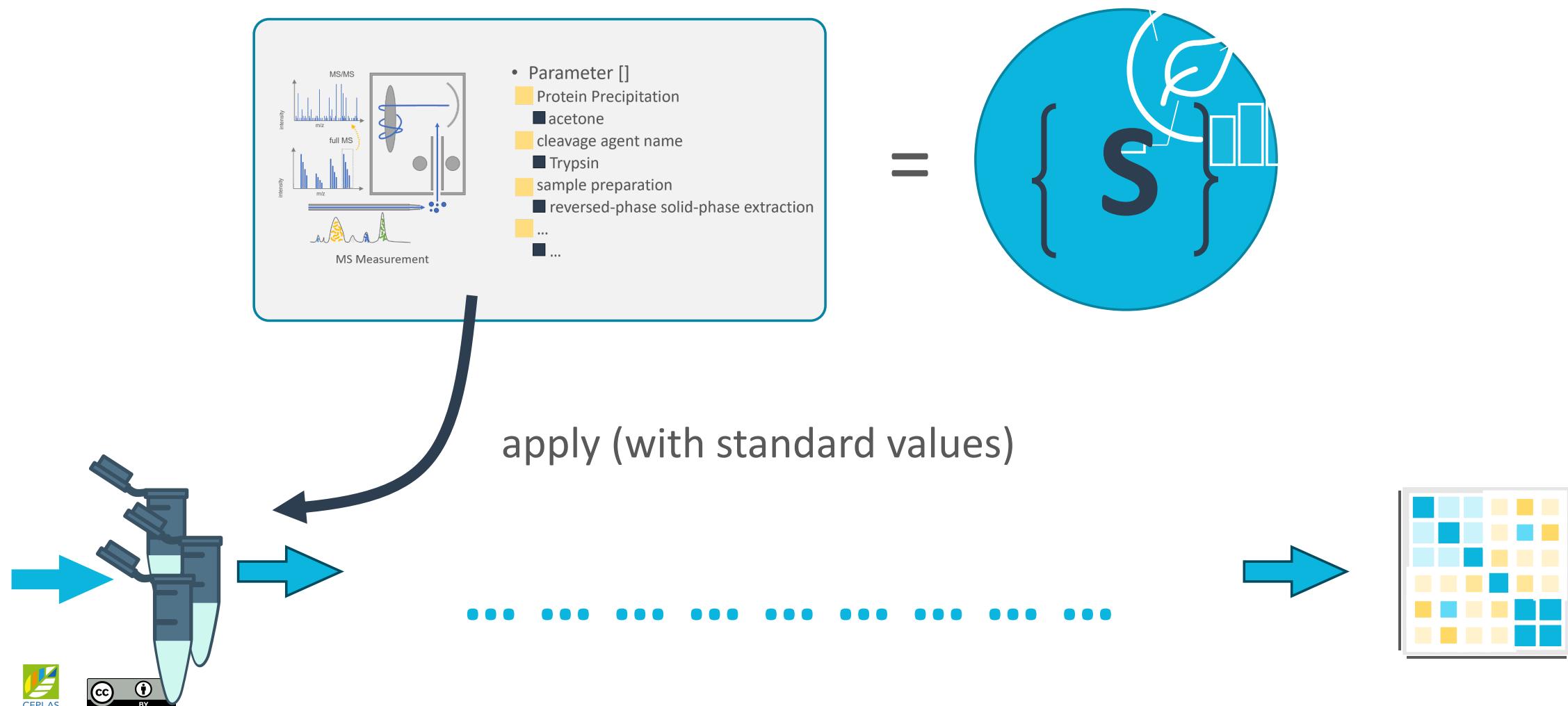
- Parameter []
 - Protein Precipitation
 - acetone
 - cleavage agent name
 - Trypsin
 - sample preparation
 - reversed-phase solid-phase extraction
 - ...
 - ...

Save time using standard methods and SOPs

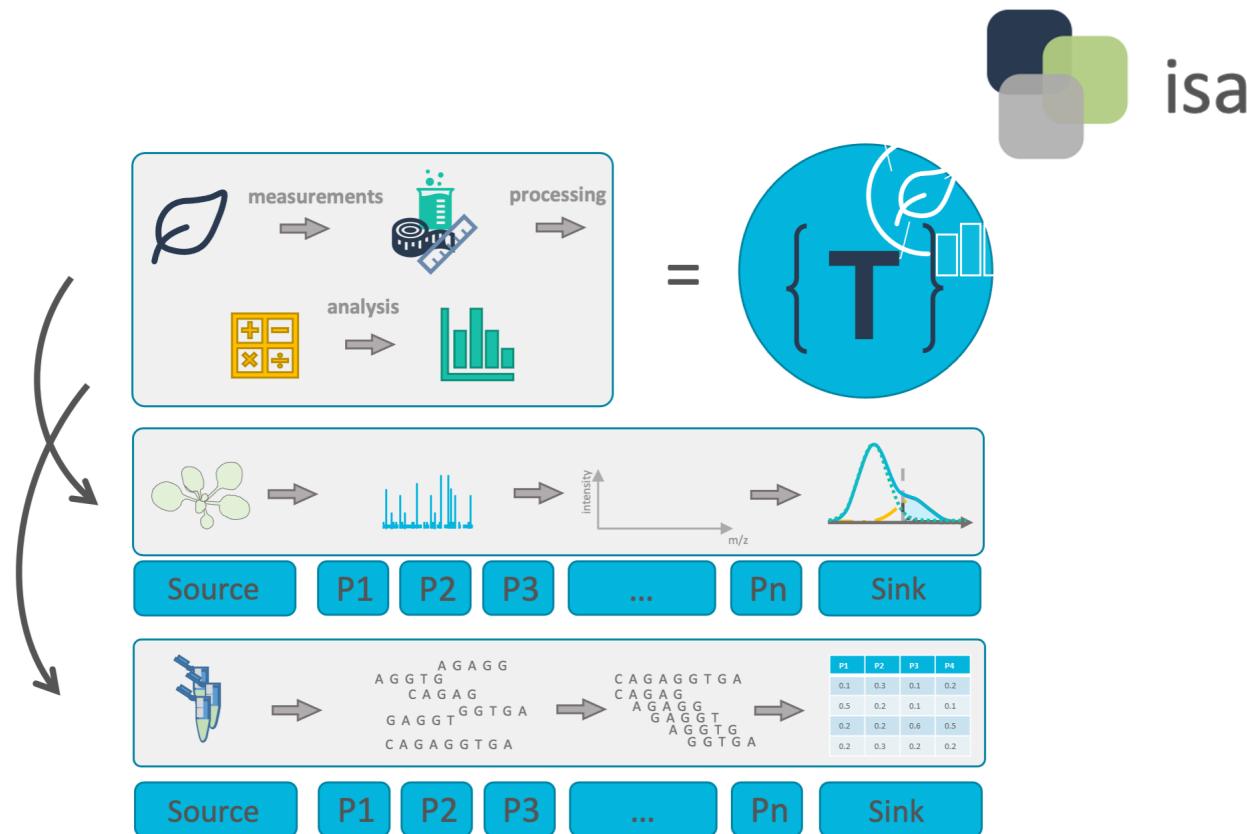


- Component []
 - chromatography instrument model
 - nanoElute2
 - chromatography column model
 - PepSep C18 1.9 μ , 25cm x 75 μ m
 - ...
 - ...
 - ...
 - ...

Applying standard procedures to sample record



Realization of lab-specific metadata templates



Facilities can define their most common workflows as templates

Import templates from a database

- DataPLANT curated
- Community templates

The screenshot shows a user interface for managing templates. At the top, there are search fields for "Search by template name" and "Search for tags", and a dropdown for "Select community" set to "DataPLANT official". Below this is a table listing various templates:

Template Name	Community	Template Version
DNA extraction	curated	1.1.7
Data Processing (PRIDE minimal)	curated	1.0.0
GEO - Minimal information RNA assays	curated	1.0.1
GEO - Minimal information RNA extraction	curated	1.0.0
GEO - Minimal information computational analysis	curated	1.0.0
GEO - Minimal information plant growth	curated	1.0.0
Genome assembly	curated	1.1.7

Let's annotate the RNA Seq assay

Open the lab notes assays/rnaseq/protocols/

Use a template

1. Open the *Templates* widget in the Bar

💡 Here you can find DataPLANT and community created workflow annotation templates

2. Search for **RNA extraction** and click **select**

- You will see a preview of all *Building Blocks* which are part of this template.

3. Click **Add template** to add all *Building Blocks* from the template to your table

The screenshot shows the 'Templates' widget interface. At the top, there are search bars for 'Search by template name' and 'Search for tags', both with placeholder text ('.. template name' and '.. protocol tag'). Below these are dropdown menus for 'Select community' (set to 'DataPLANT official') and 'Template Version'. The main area is a table listing various templates:

Template Name	Community	Template Version	Actions
DNA extraction	curated	1.1.7	▼
Data Processing (PRIDE minimal)	curated	1.0.0	▼
GEO - Minimal information RNA assays	curated	1.0.1	▼
GEO - Minimal information RNA extraction	curated	1.0.0	▼
GEO - Minimal information computational analysis	curated	1.0.0	▼
GEO - Minimal information plant growth	curated	1.0.0	▼
Genome assembly	curated	1.1.7	▼
...			...

Remove Building blocks

If there are any *Building Blocks* which do not fit to your experiment you can use right click --> "Delete Column" to remove it including all related (hidden) reference columns.

Move Building blocks

If the order of the *Building Blocks* should be adjusted you can use right click --> "Move Column"

Move Column×

Preview1ApplyUpdate TableSubmit

Index	Column
0	Input [Source Name]
1	Characteristic [Organism]
2	Factor [watering exposure]
3	Output [Sample Name]

Replace multiple names

Right click --> "Update Column" can be used to replace names in batches

 this only works on Input columns

Update Column ×

	Regex	Replacement
	DB	sample

Preview

	Before	After
0	DB_097	sample_097
1	DB_099	sample_099
2	DB_103	sample_103
3	DB_161	sample_161
4	DB_163	sample_163

Submit

New process, new worksheet

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

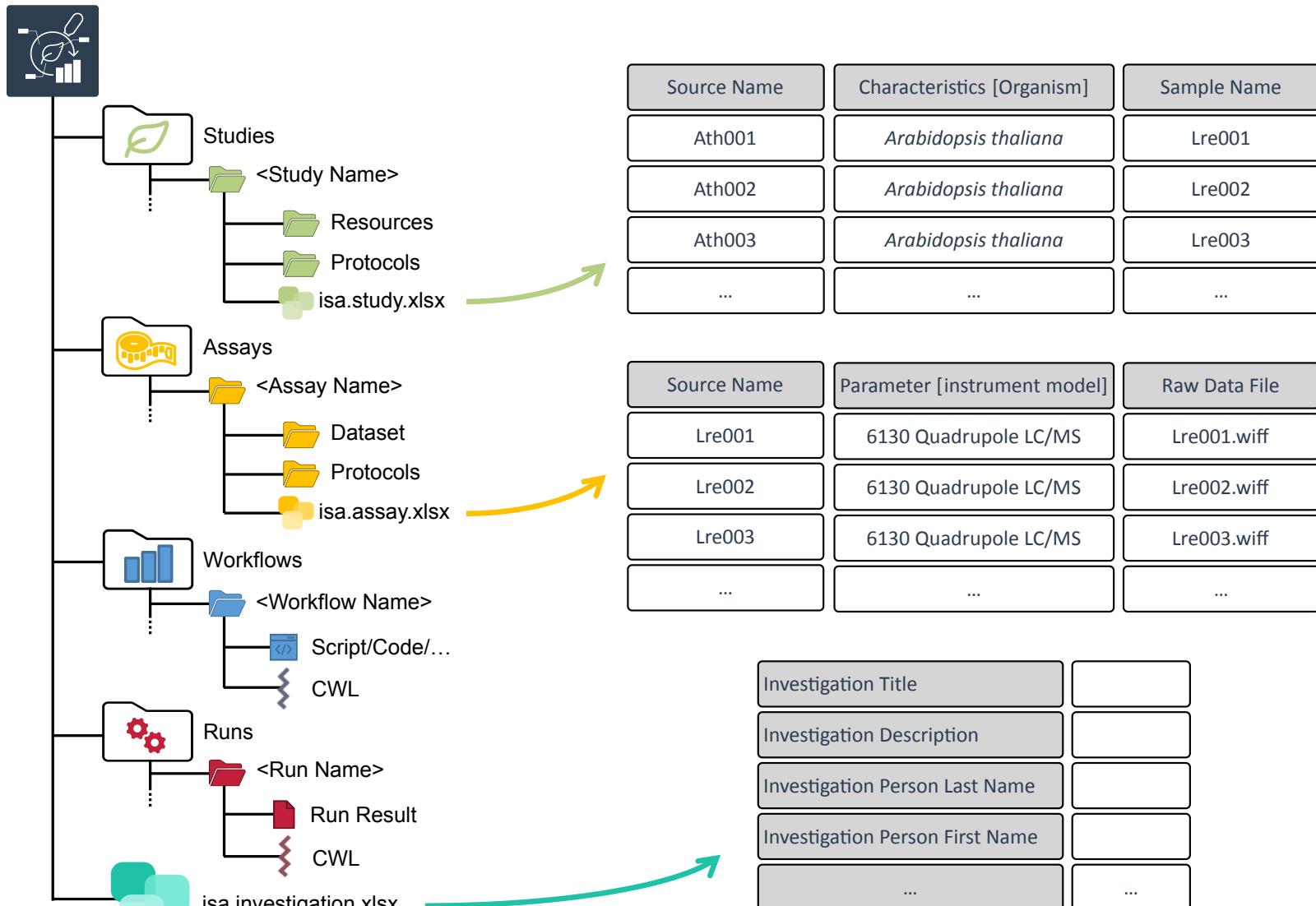
Exercise

Try to fill the two sheets with the protocol details:

- assays/rnaseq/protocols/RNA_extraction.txt and
- assays/rnaseq/protocols/Illumina_libraries.txt

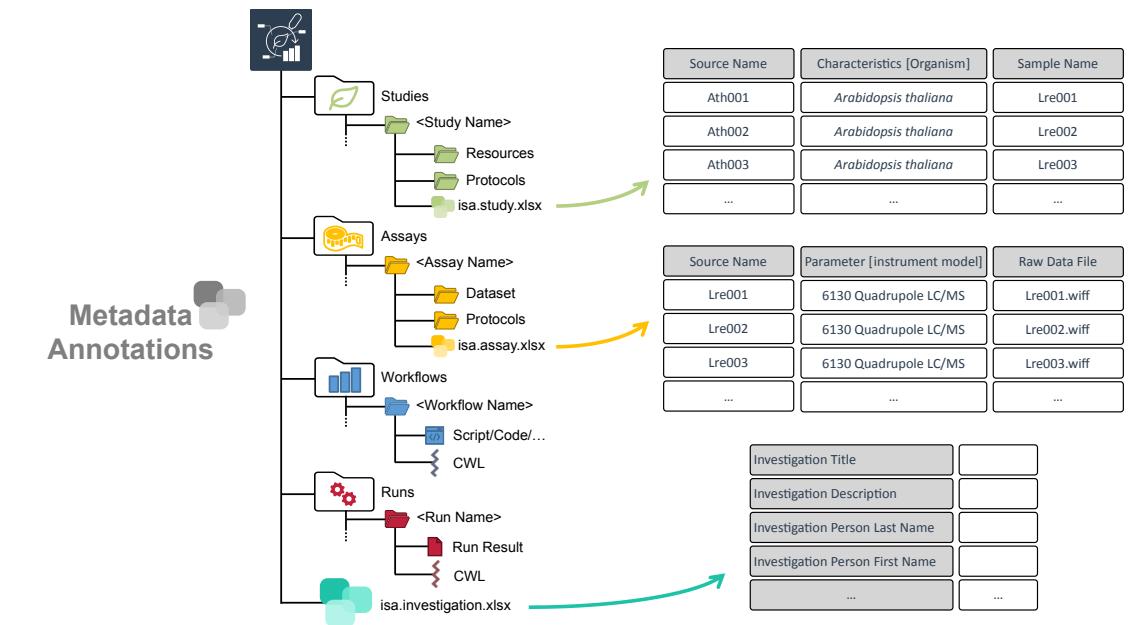
ARC builds on ISA to connect data

Metadata Annotations



ARC builds on ISA to link data

- Samples are linked study-to-assay, assay-to-assay
- Raw data is linked to assays
- Protocols can be referenced
- ...



Link samples across studies and assays

1. Use the **Output [Sample Name]** of studies/talinum_drought/isa.study.xlsx as the **Input [Sample Name]** to **rna-extraction**.
2. Use the **Output [Sample Name]** of **rna-extraction** as the **Input [Sample Name]** to **illumina-libraries**.

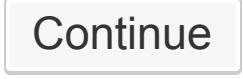
Seeds –Plant growth→ Leaves –RNA Extraction→ RNA –Illumina→ fastq files

Link dataset files to samples

1. In the *Building Blocks* widget select *Output -> Raw Data File*.

2. Click  .

 You see a warning about a changed output column.

3. Click  .

4. Go to the *File Picker* tab and click  .

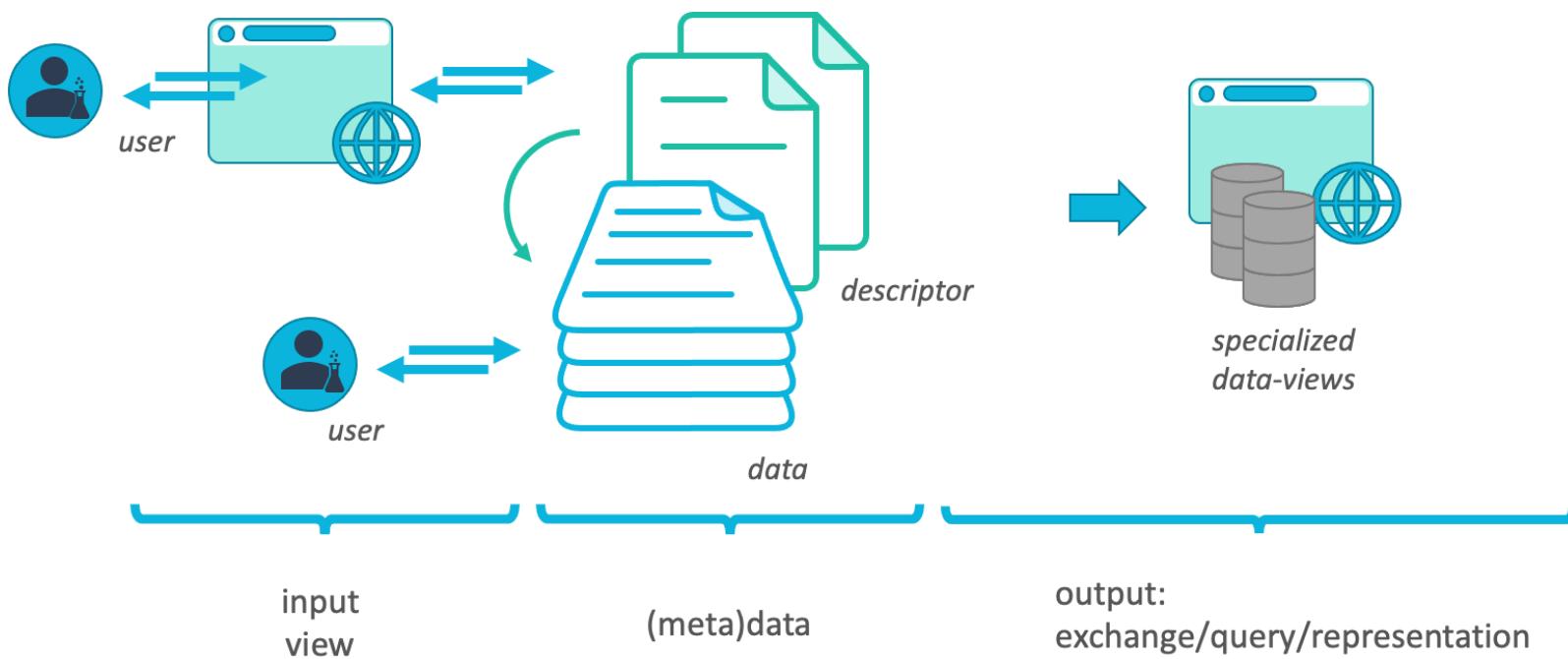
5. Select and open the *fastq.gz files from the dataset folder.

6. Copy / paste them to the  .

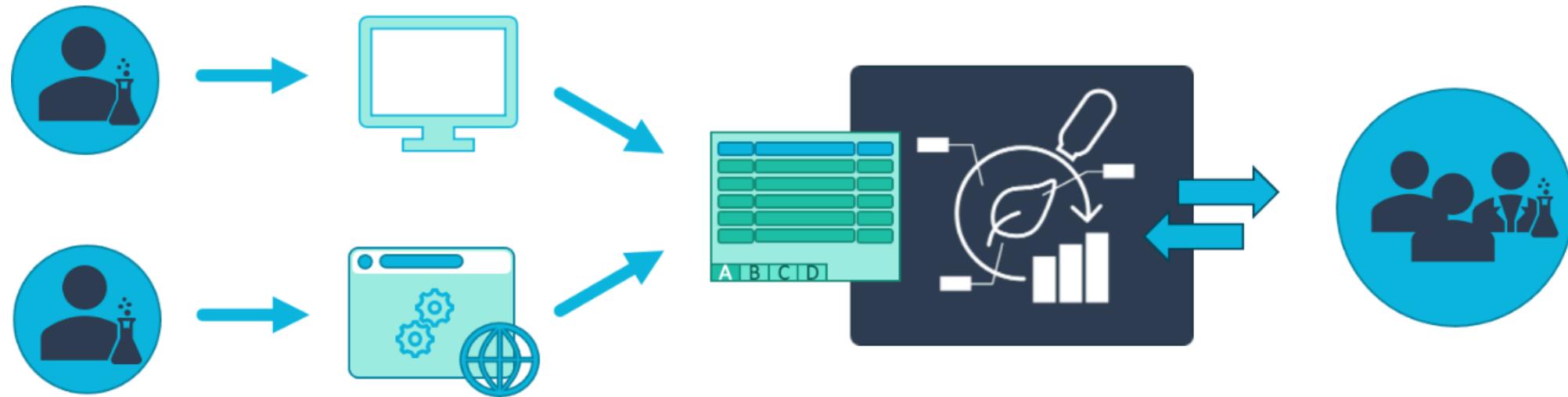
 This allows you to link your samples to the resulting raw data files.

Everything is a file

The ARC is a **data-centric** approach to RDM



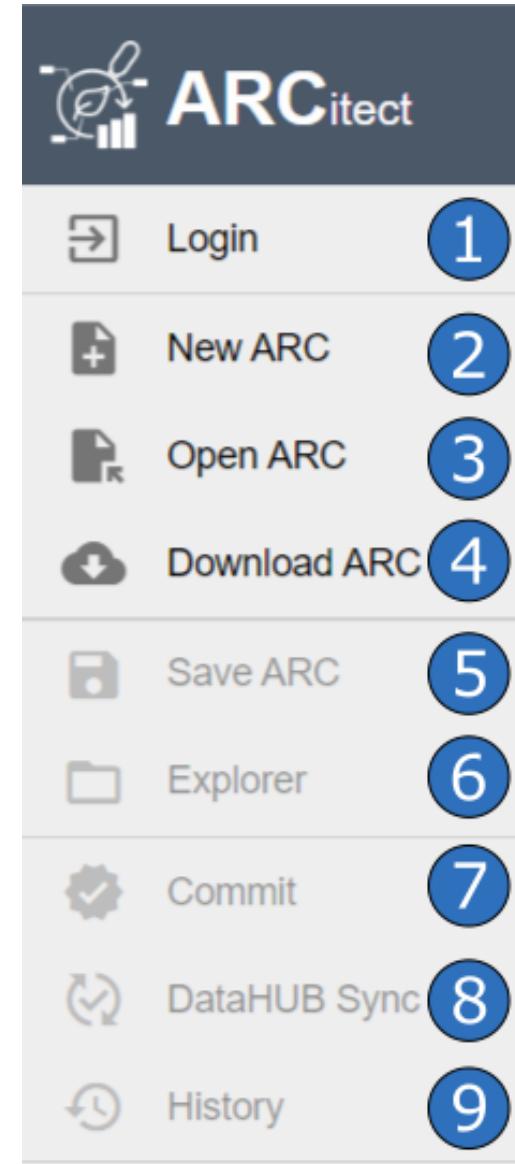
No technical lock-in



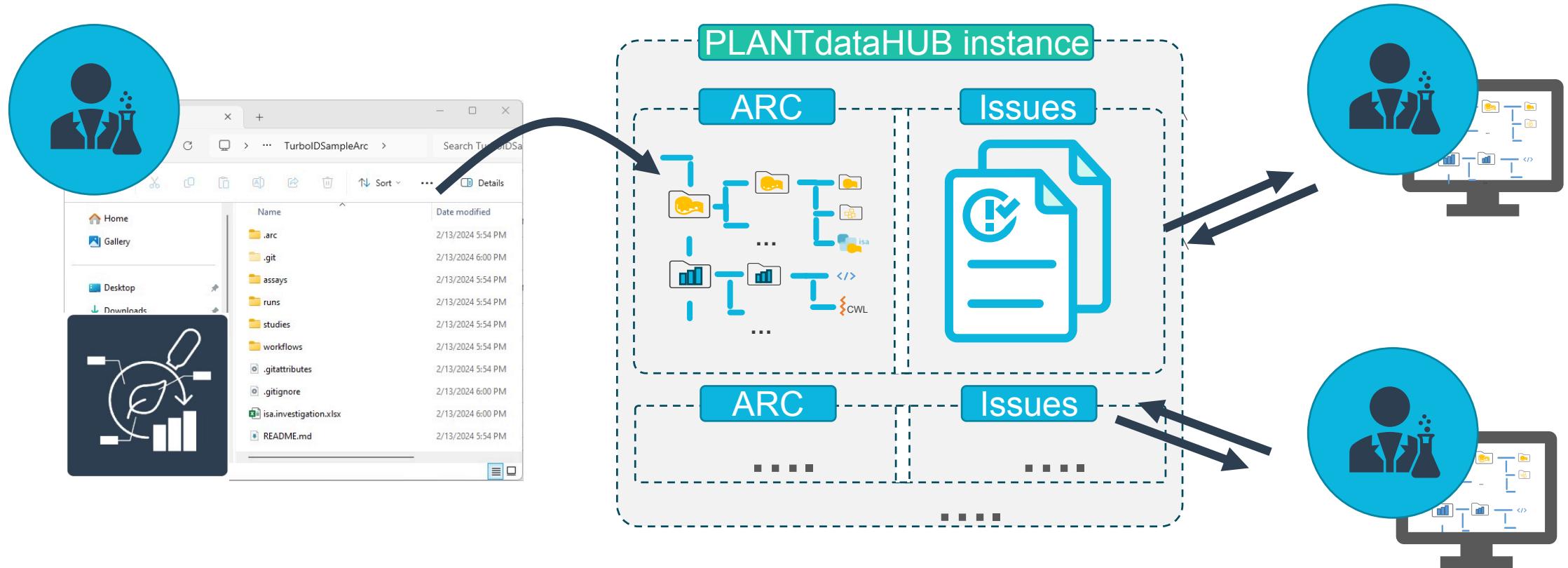
(Meta)data transparency with tool assistance but **no technical lock-in**

Explorer

The **Explorer (6)** button directly opens your ARC locally



Using the DataHUB to collaborate



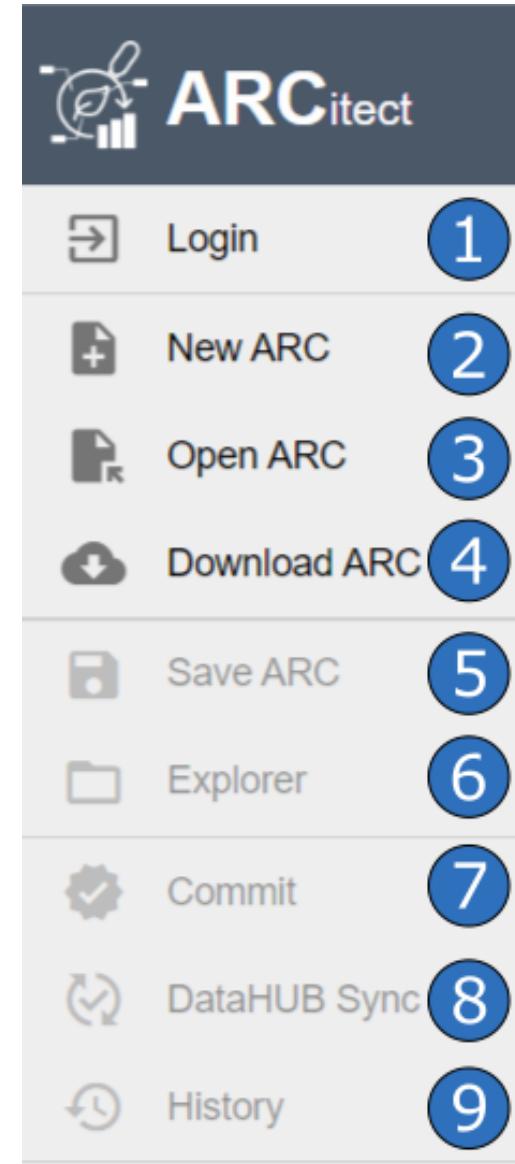
Login to DataHUB

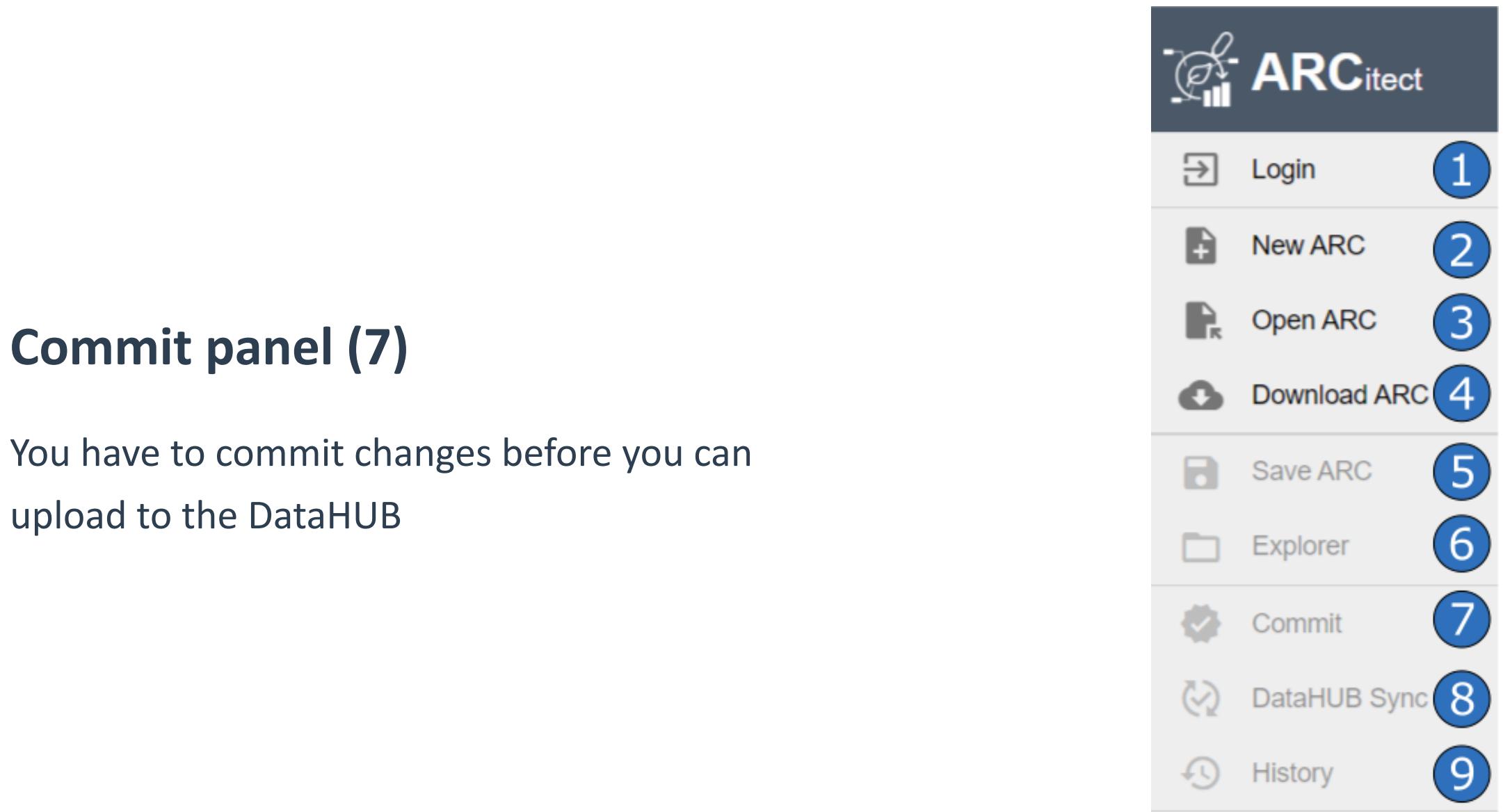
1. Login to DataHUB (1)
2. Select `git.nfdi4plants.org` as Host

Please Select a DataHub

Host
`git.nfdi4plants.org`

LOGIN CANCEL





Commit panel (7)

You have to commit changes before you can upload to the DataHUB

Commit your changes

If you are logged in, the **Commit panel** shows

- your DataHUB's *Full Name* and *eMail*

It allows you to

- track changes of the ARC with git
- add a commit message
- use different branches

The screenshot shows the 'Commit Changes' panel. At the top, it says 'Commit Changes' and 'Track changes of the ARC with git'. Below that, there are fields for 'Name' (Sabrina Zander) and 'eMail' (sabrina.zander@uni-duesseldorf.de). There are dropdowns for 'Branch' and 'Commit Message'. A field for 'Large File Storage Limit in MB' is set to 1. Below these, a section titled 'Changes' shows a message 'No changes to commit'. At the bottom are 'RESET' and 'COMMIT' buttons.

History panel (9)

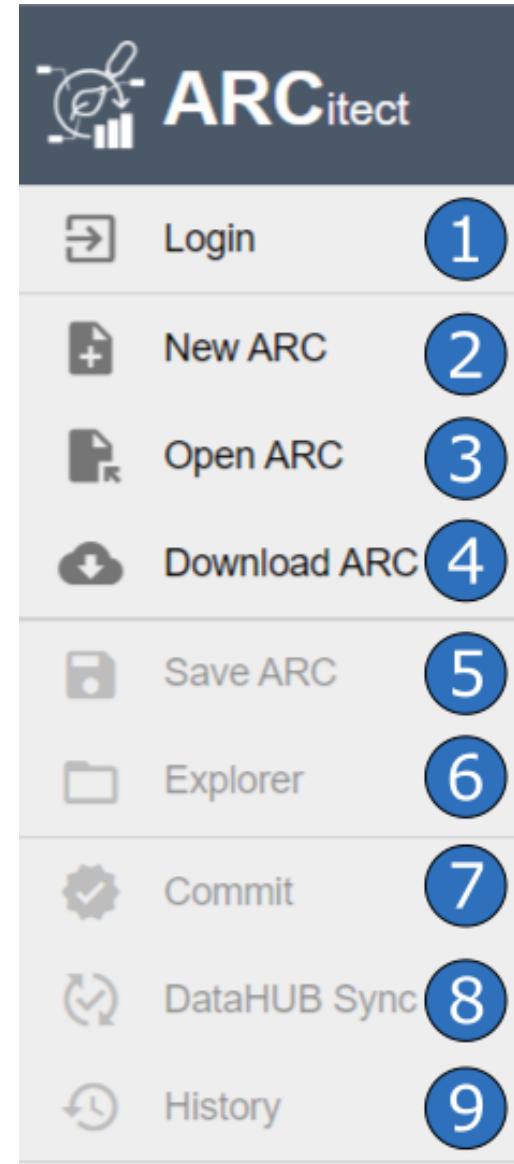
In the History panel you can inspect your ARCs history with all commits

The screenshot shows a 'History' panel with a title 'Inspect ARC history'. Below the title is a circular icon with a clock and a downward arrow. A vertical teal line represents the timeline, with six dark teal circular markers indicating commit points. To the right of each marker is a timestamp, the author's name (SABRINA ZANDER), and the email (SABRINA.ZANDER@UNI-DUESSELDORF.DE), followed by a brief description of the commit.

Date	Author	Email	Commit Description
08.04.2024 12:44	SABRINA ZANDER	SABRINA.ZANDER@UNI-DUESSELDORF.DE	add data and protocols to rnaseq
08.04.2024 12:43	SABRINA ZANDER	SABRINA.ZANDER@UNI-DUESSELDORF.DE	add assay rnaseq
08.04.2024 12:43	SABRINA ZANDER	SABRINA.ZANDER@UNI-DUESSELDORF.DE	add study talinum_drought
08.04.2024 12:43	SABRINA ZANDER	SABRINA.ZANDER@UNI-DUESSELDORF.DE	add contributors
08.04.2024 12:42	SABRINA ZANDER	SABRINA.ZANDER@UNI-DUESSELDORF.DE	add description to investigation
08.04.2024 12:41	SABRINA ZANDER	SABRINA.ZANDER@UNI-DUESSELDORF.DE	set up new ARC

Upload your local ARC to the DataHUB

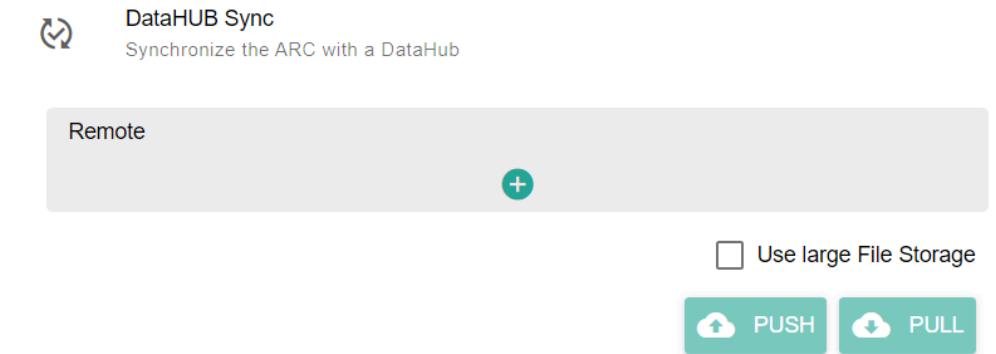
From the sidebar, navigate to **DataHUB Sync** (8)



DataHUB Sync

The DataHUB Sync panel allows you to

- sync the changes to the DataHUB: **Push**
- sync from the DataHUB: **Pull**, and
- change the Remote for the synchronization

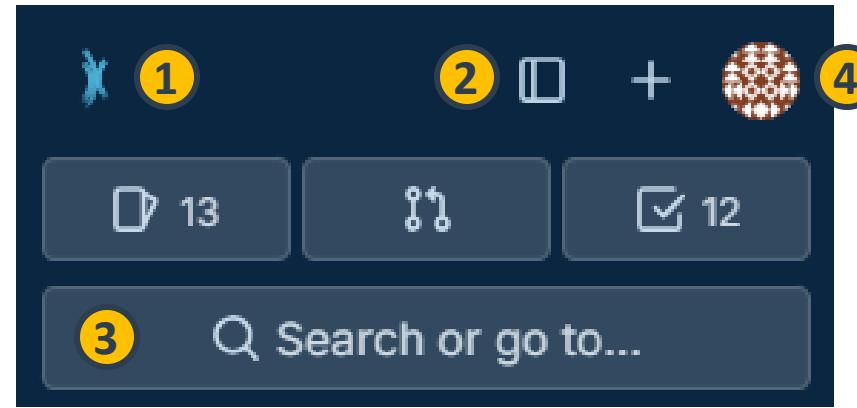


Check if your ARC is successfully uploaded

1. [sign in](#) to the DataHUB
2. Check your projects

DataHub Hands-On

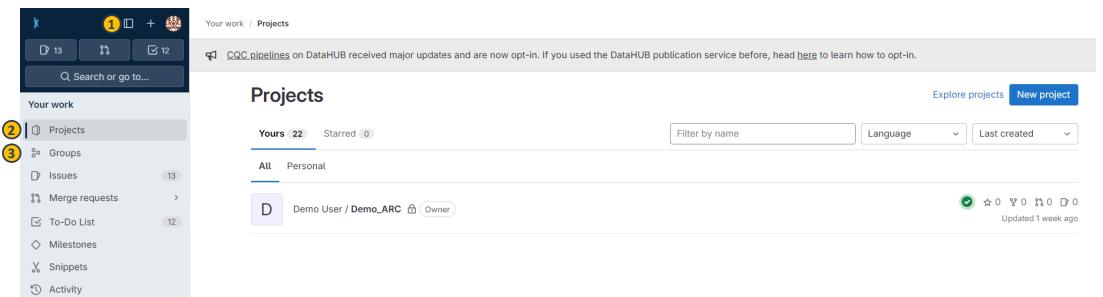
Navigation Bar



1. navigate directly to the [projects panel](#) via the icon in the top-left (1)
2. open the [hamburger Menu](#) (2)
3. use the search field (3) to find ARCs, users and groups
4. open the [avatar Menu](#) (4)

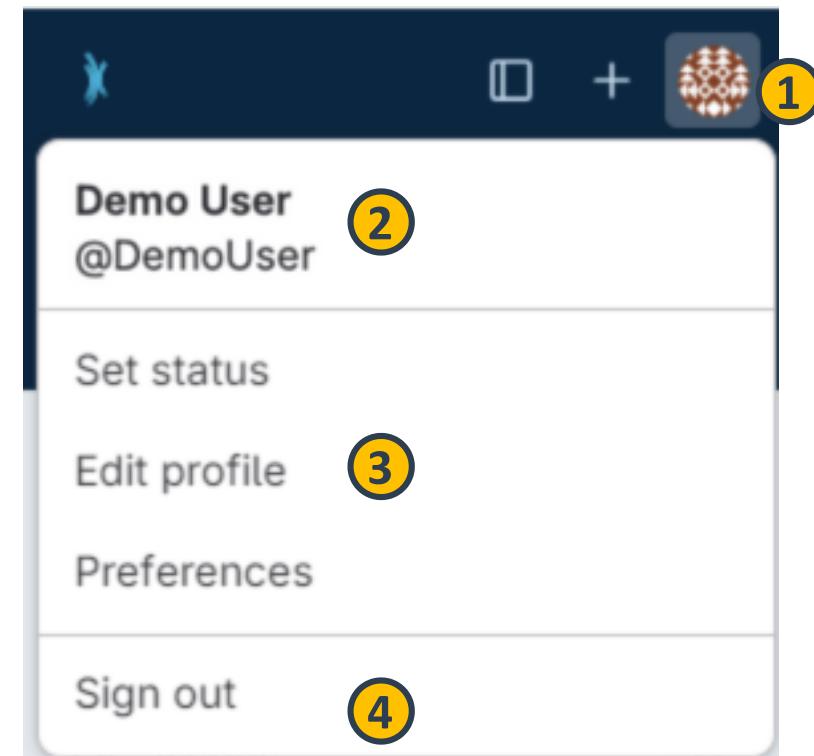
Hamburger Menu

1. From the hamburger menu (1) you can
2. navigate to the **projects** (2)
3. or **groups** (3) panels



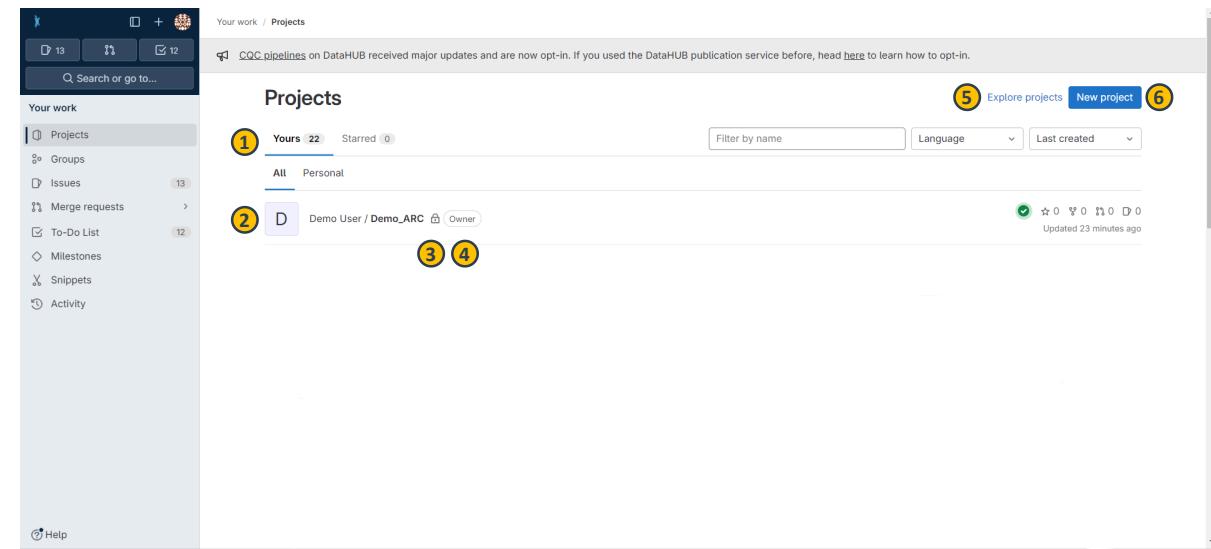
Avatar Menu

1. In the avatar menu (1) you can
2. find your profile name and user name (2),
3. navigate to the [user settings](#) (3)
4. or sign out (4) of the DataHUB.



Projects Panel

1. Choose a tab (1) to see only your ARCs, or explore other publicly available ARCs.
2. The main panel (2) lists all ARCs
3. Here you can also see, the visibility level (3), and
4. your permission or role (4) for the listed ARC.



ARC Panel

The ARC Panel is the main working area for your ARC.

The screenshot shows the DataHUB ARC Panel interface. On the left is a sidebar with navigation links: Manage (1), Plan (2), Code (3), Build (4), Secure, Deploy, Operate, Monitor, Analyze, Settings (4), and Help. The main area displays a project named "Demo_ARC" (5). The top navigation bar includes a search bar, pinned items (13, 88, 12), and a user profile icon. Below the navigation is a breadcrumb trail: Demo User / Demo_ARC. The central workspace (6) contains a file tree with "arc init" (7) and a list of files: assays, runs, studies, workflows, .gitignore, and isa.investigation.xlsx. The right side shows "Project information" (8) with a pipeline status (passed) and a "Publish ARC" button. It also lists project metrics: 1 Commit, 2 Branches, 0 Tags, and 7 KiB Project Storage. A sidebar on the far right provides links for Auto DevOps, README, LICENSE, CHANGELOG, CONTRIBUTING, Kubernetes cluster, Wiki, and Configure Integrations. At the bottom are footer links for DataPLANT, CEPLAS, CC BY, and a page number 109.

Demo User / Demo_ARC

D Demo_ARC locked (5)

main Demo_ARC / + (7)

arc init
Demo User authored 4 minutes ago

Name Last commit Last update

assays	arc init	4 minutes ago
runs	arc init	4 minutes ago
studies	arc init	4 minutes ago
workflows	arc init	4 minutes ago
.gitignore	arc init	4 minutes ago
isa.investigation.xlsx	arc init	4 minutes ago

Project information

pipeline passed Published Publish ARC

1 Commit

2 Branches

0 Tags

7 KiB Project Storage

Auto DevOps enabled

+ Add README

+ Add LICENSE

+ Add CHANGELOG

+ Add CONTRIBUTING

+ Add Kubernetes cluster

+ Add Wiki

+ Configure Integrations

Created on

July 13, 2024

DataPLANT CEPLAS CC BY

109

ARC Panel – sidebar

1. access the project information (1), e.g.
invite members to the ARC
2. follow the progress of your ARC
repository (2),
3. organize tasks in issue lists and boards
(3),
4. take notes in a wiki to your ARC (4),
5. adapt the **settings** (5) of the ARC.

The screenshot shows the DataHUB interface. On the left is a sidebar with navigation items: Manage (1), Plan (2), Code (3), Build (4), Secure (5), Deploy (6), Operate (7), Monitor (8), Analyze (9), Settings (10), and Help (11). The main area displays project details for 'Demo User / Demo_ARC'. It includes a commit history table:

Name	Last commit	Last update
assays	arc init	4 minutes ago
runs	arc init	4 minutes ago
studies	arc init	4 minutes ago
workflows	arc init	4 minutes ago
.gitignore	arc init	4 minutes ago
isa.investigation.xlsx	arc init	4 minutes ago

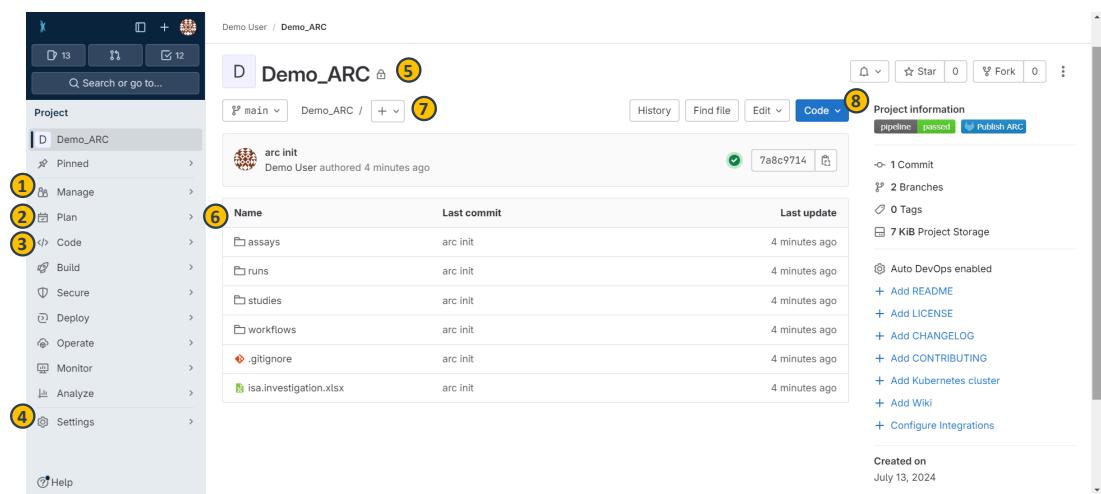
On the right, the 'Project information' section shows:

- pipeline: passed
- 1 Commit
- 2 Branches
- 0 Tags
- 7 KIB Project Storage
- Auto DevOps enabled
- + Add README
- + Add LICENSE
- + Add CHANGELOG
- + Add CONTRIBUTING
- + Add Kubernetes cluster
- + Add Wiki
- + Configure Integrations

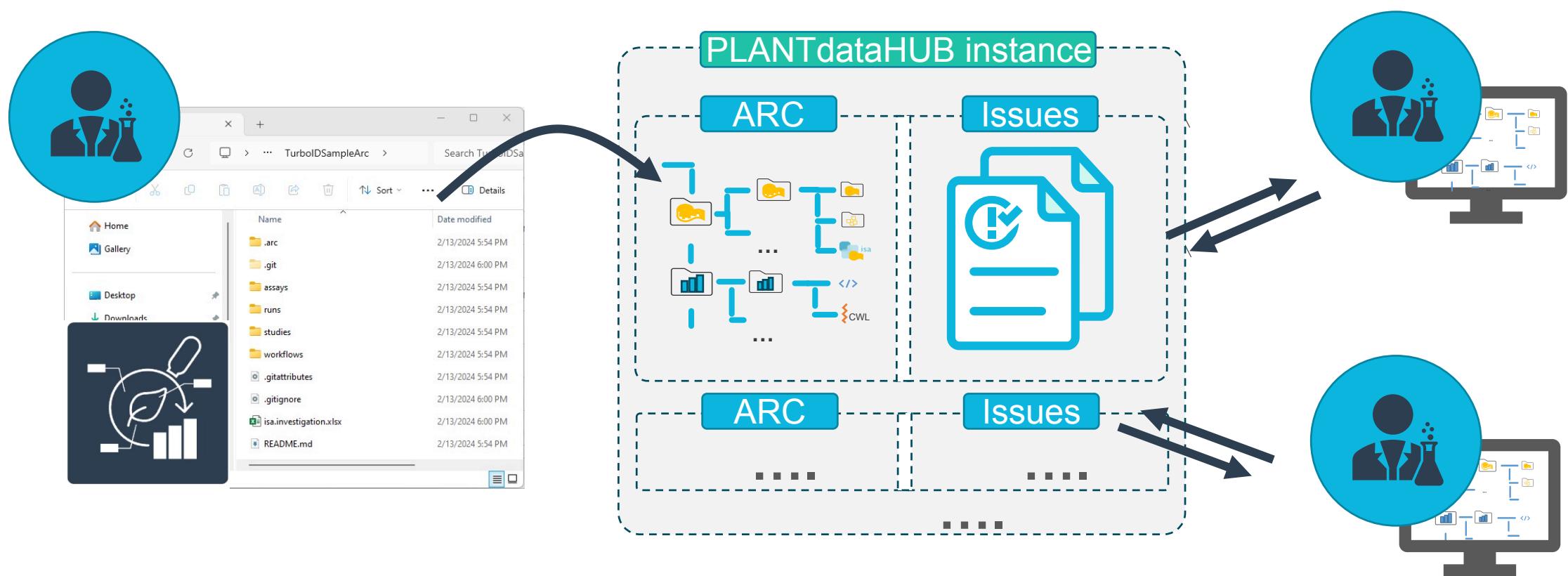
At the bottom, it says 'Created on July 13, 2024'.

ARC Panel – main panel

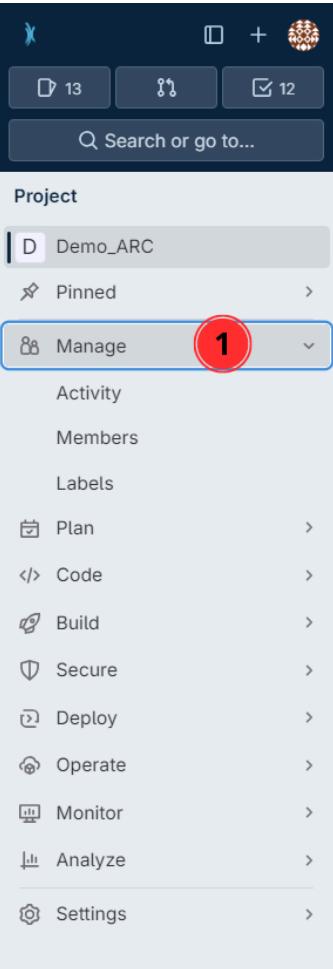
6. see the ARC's name and visibility level (6),
7. follow the ARC's commit history (7),
8. see files contained in your ARC just like on your computer (8),
9. add new files or directories (9), and
10. download or clone your ARC (10).



Collaborate and share



1. Click on Project Information in the left navigation panel



The screenshot shows the DataHUB web interface. On the left, there is a navigation sidebar with various project management options like Plan, Code, Build, Secure, Deploy, Operate, Monitor, Analyze, and Settings. The 'Manage' option is highlighted with a red circle and has a count of 1 next to it. The main content area shows a project named 'Demo_ARC'. At the top right of the main area, there are buttons for 'History', 'Find file', 'Edit', 'Code' (which is currently selected), 'Project information', 'pipeline passed', and 'Publish ARC'. Below this, there is a commit history table and a detailed view of a single commit. To the right of the commit history, there is a sidebar titled 'Project information' containing various project statistics and configuration links.

Demo User / Demo_ARC

CQC pipelines on DataHUB received major updates and are now opt-in. If you used the DataHUB publication service before, head [here](#) to learn how to opt-in.

D Demo_ARC

main Demo_ARC / +

History Find file Edit Code

Project information

pipeline passed Publish ARC

1 Commit

2 Branches

0 Tags

21 KiB Project Storage

Auto DevOps enabled

Wiki

Add README

Add LICENSE

Add CHANGELOG

Add CONTRIBUTING

Add Kubernetes cluster

Configure Integrations

Created on July 13, 2024

Name	Last commit	Last update
assays	arc init	1 week ago
runs	arc init	1 week ago
studies	arc init	1 week ago
workflows	arc init	1 week ago
.gitignore	arc init	1 week ago
isa.investigation.xlsx	arc init	1 week ago

arc init
Demo User authored 1 week ago

7a8c9714

2. Click on Members

The screenshot shows the DataHUB interface for a project named 'Demo_ARC'. On the left, there is a sidebar with various project management options like Plan, Code, Build, Secure, Deploy, Operate, Monitor, Analyze, and Settings. Two specific items are highlighted with red circles and numbers: 'Manage' (number 1) and 'Members' (number 2). The main content area is titled 'Project members' and displays a single member named 'Demo User' (@DemoUser). The member is listed under the 'Members' tab, which has a count of 1. There is also a 'Pinned' item in the sidebar.

Demo User / Demo_ARC / Members

CQC_pipelines on DataHUB received major updates and are now opt-in. If you used the DataHUB publication service before, head [here](#) to learn how to opt-in.

Project members

You can invite a new member to Demo_ARC or invite another group.

Members 1

Filter members Account ▾

Account	Source	Max role	Expiration	Activity
 Demo User @DemoUser It's you	Direct member by Demo User	Owner	Expiration date 8+ Sep 27, 2023	✓ Jul 13, 2024 ✗ Jul 21, 2024

Import from a project Invite a group Invite members

3. Click on Invite members

The screenshot shows the DataHUB interface for a project named 'Demo_ARC'. The left sidebar has a 'Members' tab selected (labeled 2). The main area shows 'Project members' with one member listed: 'Demo User @DemoUser' (labeled 1). A red circle highlights the 'Invite members' button in the top right corner of the main content area (labeled 3).

Account	Source	Max role	Expiration	Activity
Demo User @DemoUser <i>It's you</i>	Direct member by Demo User	Owner	8+ Sep 27, 2023 ✓ Jul 13, 2024 ✗ Jul 21, 2024	⋮

4. Search for potential collaborators

Invite members X

You're inviting members to the **Demo_ARC** project.

Username, name or email address 4

Select members or type email addresses

Select a role

Guest ▼

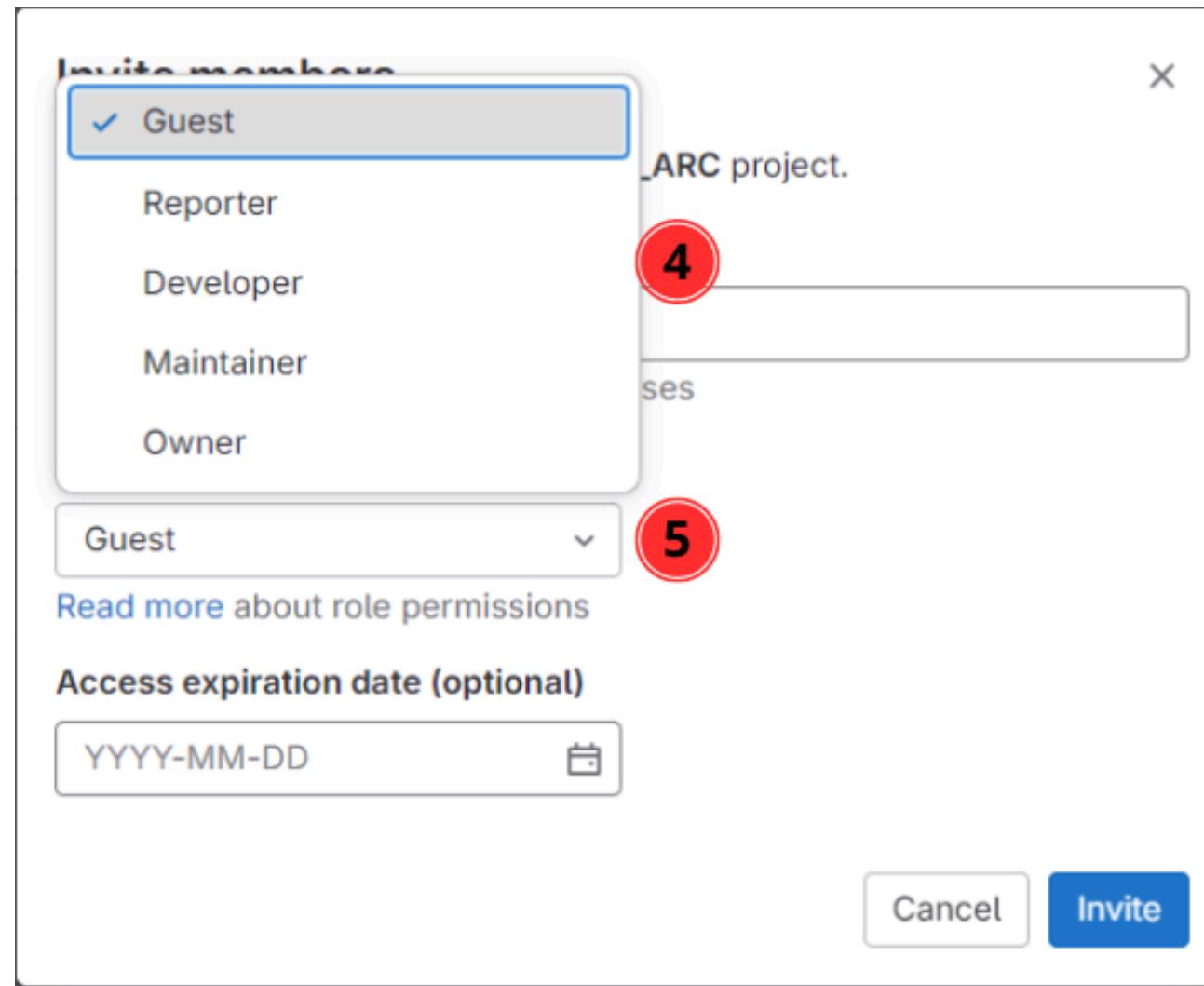
[Read more](#) about role permissions

Access expiration date (optional)

YYYY-MM-DD ▼

Cancel Invite

5. Select a role



Choosing the proper role

When inviting new members to an ARC or group, you can choose between different levels.

Permissions & Roles

Roles are assigned when adding a user to an ARC or to a group. This is a very simplified summary.

Guest – Can only see the ARC's wiki

Reporter – Can read, but not add or edit data

Developer – Reporter permissions + can read, add, and edit data

Maintainer – Developer permissions + can add new members

Owner – Maintainer + can delete ARC, manage memberships and permissions

 By default you are **Owner** of an ARC you create or upload to the DataHUB.

Projects and Groups are not the same

- "Project" = ARC
- "Groups" = Group of users

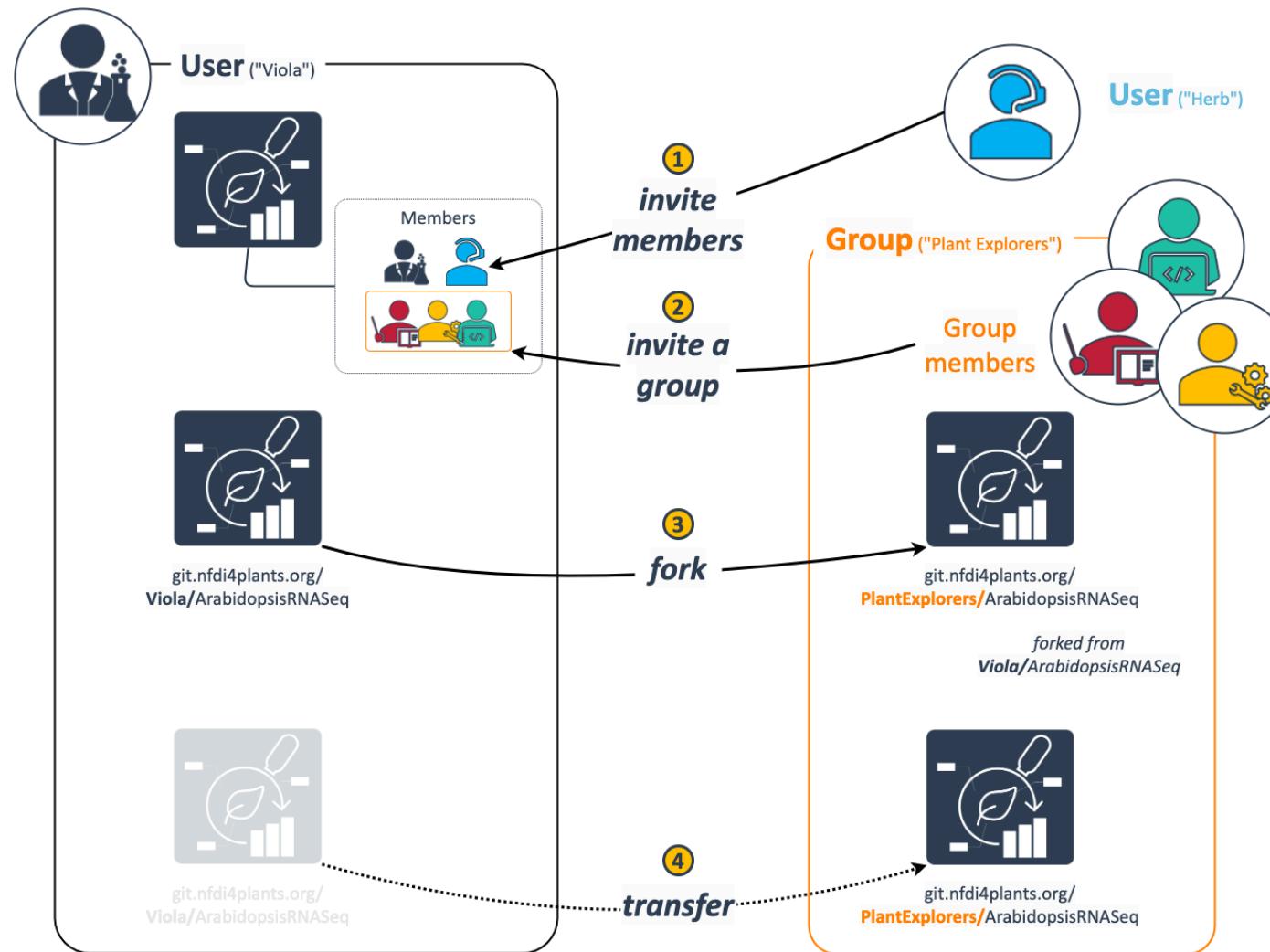
Project = ARC

- In the DataHUB, ARCs are called "projects"; they are the same.
- An ARC can be shared with individual users (invited as "members") or a group.

DataHUB Groups = Group of members (e.g. lab)

- A "Group" is a group of users with specific permissions
- A group can share ARCs
- A group can be invited to an ARC
- Groups can have subgroups

Options to share an ARC via the DataHUB



Namespaces

- Every user has a personal namespace, where they can upload or create new ARCs
- Every group and subgroup has its own namespace

Type	URL	Namespace	Name
A personal ARC	https://git.nfdi4plants.org/brilator/Facultative-CAM-in-Talinum	brilator	Dominik Brilhaus
An group-shared ARC	https://git.nfdi4plants.org/hhu-plant-biochemistry/Samuilov-2018-BOU-PSP	hhu-plant-biochemistry	HHU Plant Biochemistry

 **Personal** is not the same as **private**

Visibility

The visibility of ARCs and groups can be managed individually for each ARC or group

Visibility

The visibility of each ARC can be managed in the settings of the ARC



Private – ARC access must be granted explicitly to each user or group.



Internal – ARC can be accessed by any logged in user.



Public – ARC can be accessed without authentication.



By default every ARC and every group is set to **private**.

ARC DataHUB members // ARC Investigation contacts

The screenshot shows the 'Members' section of a GitLab project named 'Samuilov-2018-BOU-PSP'. It lists four project members:

Account	Source	Max role	Expiration	Activity
Adriano Nunes-Nesi @nunesnesi	HHU Plant Biochemistry by Sebastian Triesch	Maintainer	Expiration date	User created: Jul 05, 2023 Access granted: Jul 10, 2023 Last activity: Aug 09, 2023
Andreas Weber @andreas.weber	HHU Plant Biochemistry by Sebastian Triesch	Maintainer	Expiration date	User created: Mar 10, 2023 Access granted: Jul 31, 2023 Last activity: Sep 11, 2023
Dominik Brilhaus It's you @brilator	Direct member by Dominik Brilhaus	Owner	Expiration date	User created: Feb 21, 2022 Access granted: Dec 06, 2023 Last activity: Mar 26, 2024
Franziska Fichtner @franziska.fichtner	HHU Plant Biochemistry by Sebastian Triesch	Maintainer	Expiration date	User created: Aug 11, 2023 Access granted: Aug 11, 2023 Last activity: Aug 11, 2023

DataHUB: ARC members

https://git.nfdi4plants.org/hhu-plant-biochemistry/Samuilov-2018-BOU-PSP/-/project_members

The screenshot shows the 'Investigation Contacts' section of the ARCIctect interface for the 'Samuilov-2018-BOU-PSP' project. It lists ten contacts with their ORCID IDs and scores:

Contact	Score
Sladjana Samuilov <orcid>	4/10
Nadine Rademacher <orcid>	3/10
Samantha Flachbart <orcid>	3/10
Leila Arab <orcid>	3/10
Saleh Alfarraj <orcid>	3/10
Franziska Kuhnert <orcid>	3/10
Stanislav Kopriva <orcid>	3/10
Andreas P. M. Weber <orcid>	4/10
Tabea Mettler-Altmann <orcid>	3/10

ARCIctect: Investigation Contacts

Investigation contacts are not automatically invited as members to the ARC.

Version control

Check out the **commit history** of your ARC via Repository (2) or directly via commits (7)

The screenshot shows the DataHUB interface with the following numbered callouts:

- 1** Manage: Project management menu.
- 2** Plan: Plan section.
- 3** Code: Code section.
- 4** Settings: Settings menu.
- 5** Demo_ARC: Project name in the header.
- 6** Name: Column header for the file list table.
- 7** History: History tab in the repository view.
- 8** Project information: Project information sidebar.

Demo User / Demo_ARC

D Demo_ARC **5**

main Demo_ARC / **7**

arc init Demo User authored 4 minutes ago **8**

Name	Last commit	Last update
assays	arc init	4 minutes ago
runs	arc init	4 minutes ago
studies	arc init	4 minutes ago
workflows	arc init	4 minutes ago
.gitignore	arc init	4 minutes ago
isa.investigation.xlsx	arc init	4 minutes ago

Project information

pipeline passed **8** Publish ARC

-o 1 Commit
2 Branches
0 Tags
7 KiB Project Storage

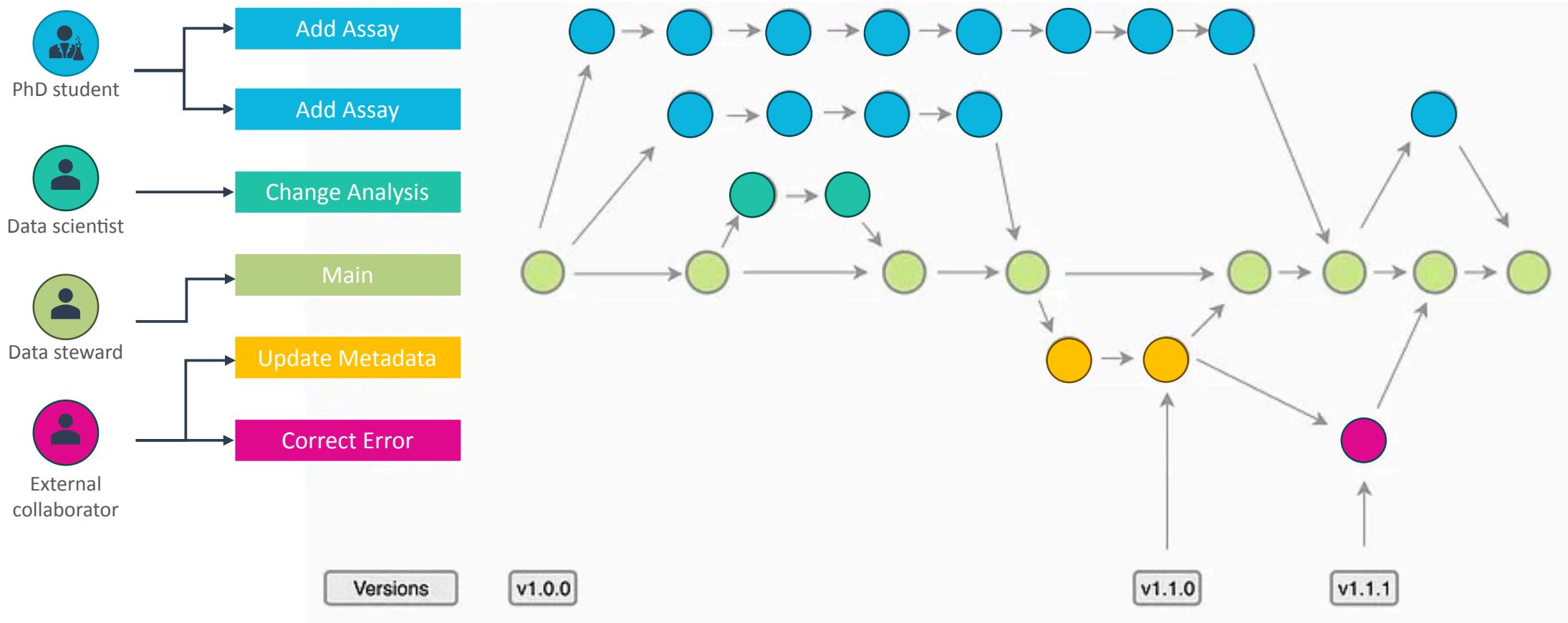
Auto DevOps enabled

+ Add README
+ Add LICENSE
+ Add CHANGELOG
+ Add CONTRIBUTING
+ Add Kubernetes cluster
+ Add Wiki
+ Configure Integrations

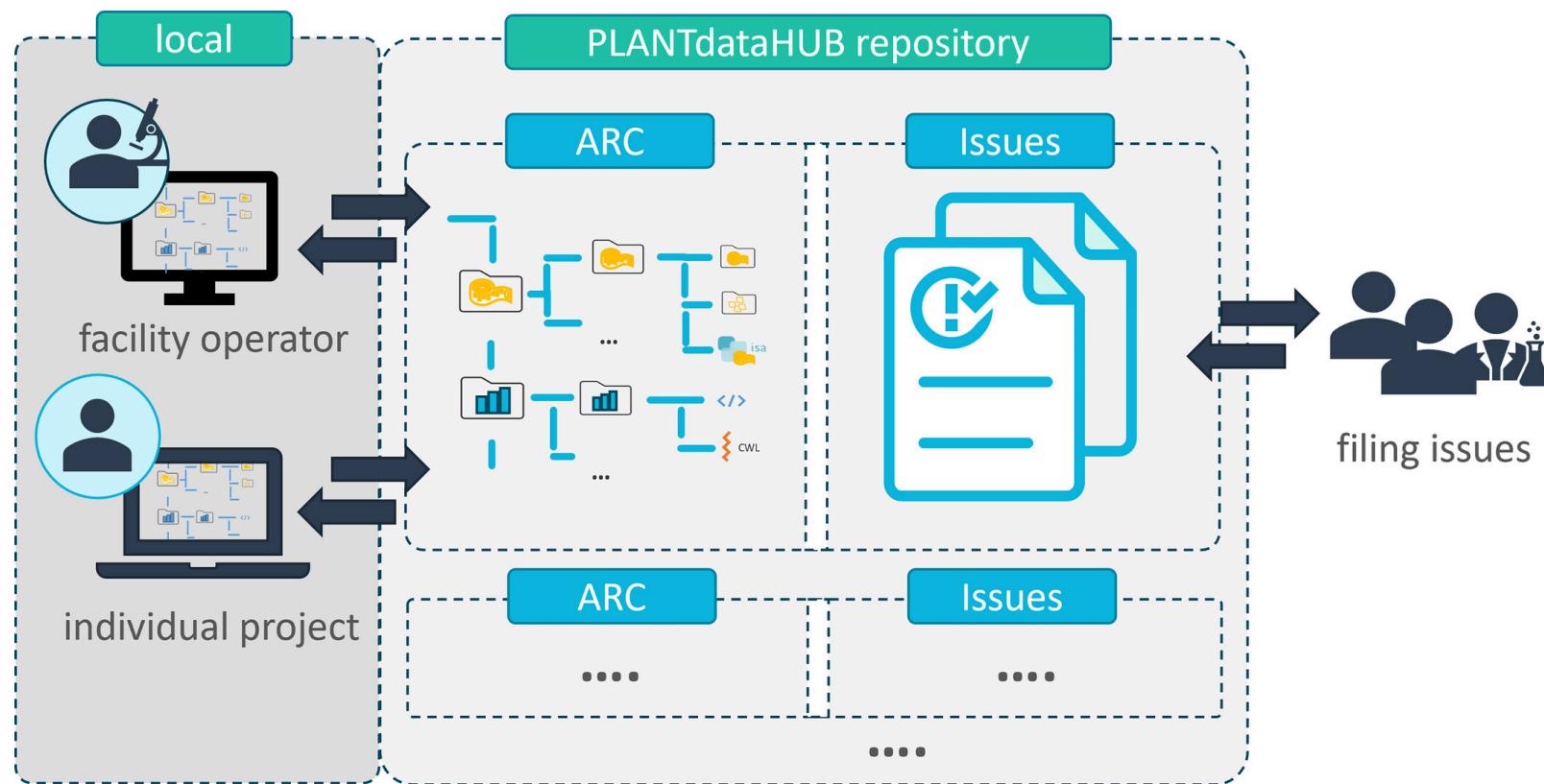
Created on July 13, 2024

Data PLANT CEPLAS CC BY

Collaboration Workflows



Project management



Project Management

Add issues to your ARC (3)

The screenshot shows the DataHUB Project Management interface. On the left, there is a sidebar with various project management options: Manage (1), Plan (2), Code (3), Build, Secure, Deploy, Operate, Monitor, Analyze, Settings (4), and Help. The main workspace is titled "Demo User / Demo_ARC". It displays a file tree under "arc init" with the following structure:

Name	Last commit	Last update
assays	arc init	4 minutes ago
runs	arc init	4 minutes ago
studies	arc init	4 minutes ago
workflows	arc init	4 minutes ago
.gitignore	arc init	4 minutes ago
isa.investigation.xlsx	arc init	4 minutes ago

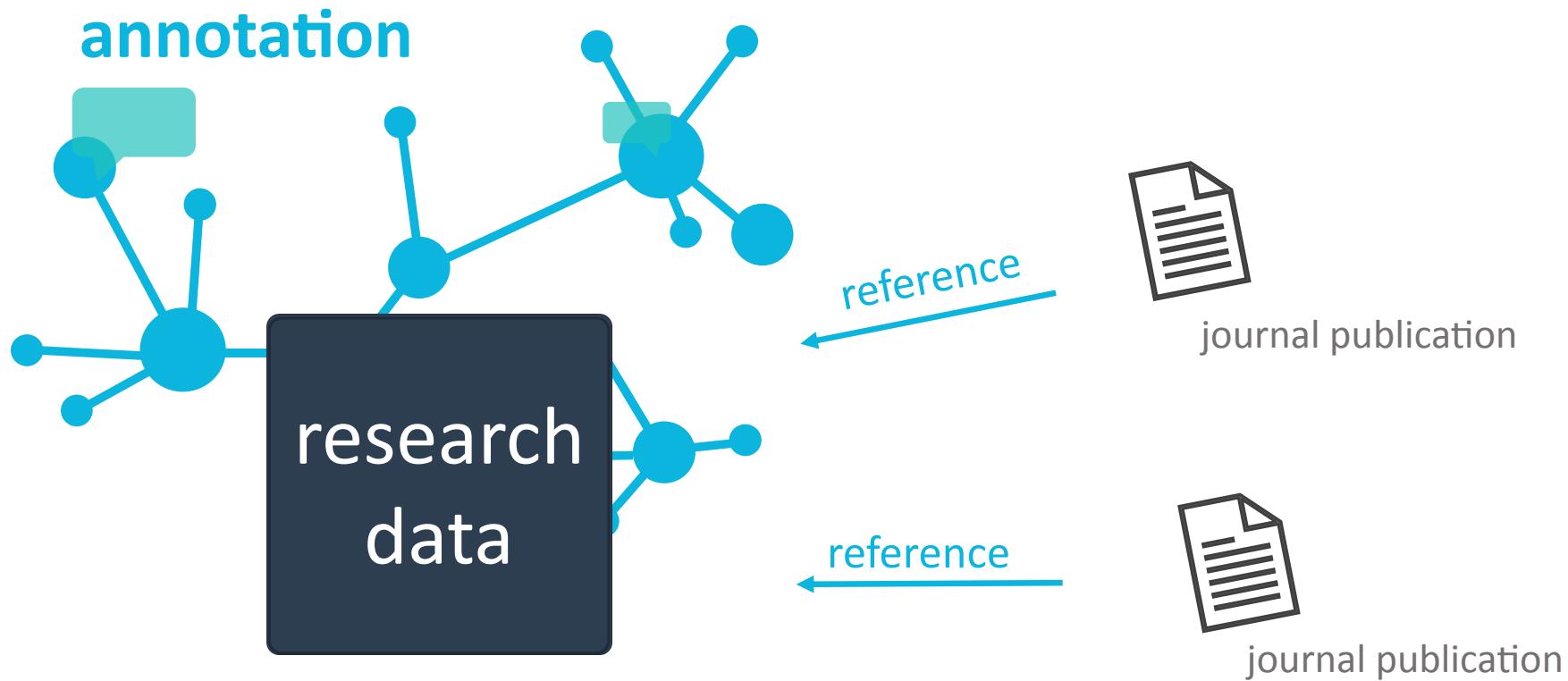
At the top right, there are buttons for History, Find file, Edit, Code (selected), and Project information. The Project information section shows a green "pipeline passed" status and a blue "Publish ARC" button. Below this, it lists 1 Commit, 2 Branches, 0 Tags, and 7 KiB Project Storage. There are also links to Auto DevOps enabled and various integration options like Add README, Add LICENSE, etc.

ARCs come with their own wiki space

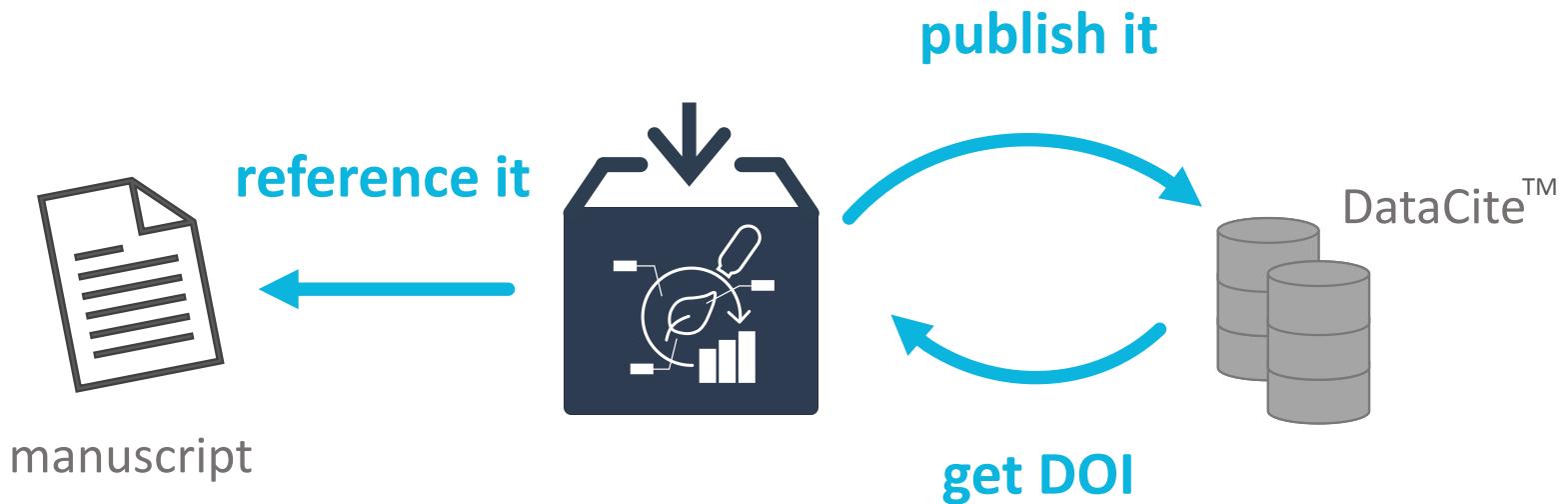
- directly associated to your ARC
- same access rights as your ARC
- share meeting minutes or ideas with collaboration partners
- keep ARC clean of files that are not considered "research data"

The screenshot shows the DataHUB interface. On the left, a sidebar for the 'Demo_ARC' project is visible, featuring sections for Project (with 'Demo_ARC' pinned), Manage, Plan, Issues (0), Issue boards, Milestones, and Wiki. The Wiki section is currently selected. The main content area displays a 'Home' page for the 'Wiki' of 'Demo_ARC'. The page header includes the URL 'Demo User / Demo_ARC / Wiki / Home'. A note at the top states: 'QC.pipelines on DataHUB received major updates and are now opt-in. If you used the DataHUB publication service before, head [here](#) to learn how to opt-in.' Below this is a 'Home' section with a 'Last edited by Demo User just now' message and a note: 'This is the wiki to Demo_ARC. We will announce meeting schedules here.' To the right of the home page, there is a sidebar titled 'Pages 2' with a 'Meeting Schedule' and 'Ideas and drafts' section.

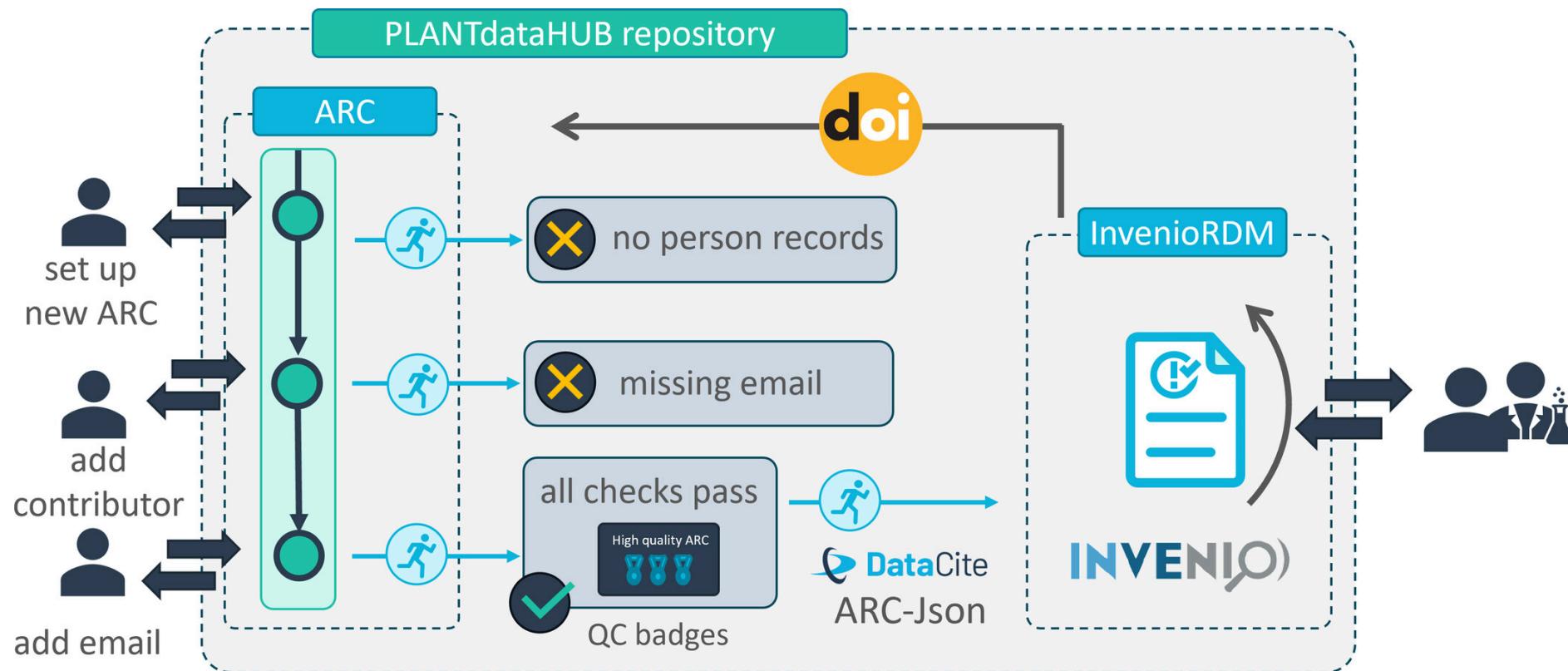
Moving from paper to FAIR data publication



Publish your ARC, get a DOI



Validate & publish



Validation towards publication

 **Ru_ChlamyHeatstress** 

 **add validation_packages.yml**
Kevin Schneider authored 2 months ago

History Find file Code

Name	Last commit	Last update
.arc	add validation_packages.yml	2 months ago
assays	Add missing data files	1 year ago
publication	add publication, add zScores	2 years ago
runs	add tpm data	1 year ago
studies	add publication information	1 year ago
workflows	Update	2 years ago
.gitattributes	rename missing samples; #2	1 year ago
.gitignore	add gitignore	1 year ago
README.md	Add doi badge	1 year ago
isa.investigation.xlsx	add author emails and adapt title	1 year ago

 README.md

Project information

Algae cultures were grown mixotrophically (TAP). After 24h of 35°C/40°C the cells were shifted back to room temperature for 48h. 'omics samples were taken.

Chlamydomonas abiotic stress
proteomics + 1 more

pipeline passed invenio 10/10

-o 55 Commits
2 Branches
0 Tags

 README
Auto DevOps enabled

Created on
July 11, 2022





Chlamydomonas reinhardtii heat stress time course experiment

Receive a DOI

Published September 7, 2023 | Version v1

Dataset 

Systems-wide investigation of responses to moderate and acute high temperatures in the green alga Chlamydomonas reinhardtii.

Zhang, Ningning¹; Mattoon, Erin¹; McHargue, Will¹ ; Venn, Benedict² ; Zimmer, David² ; Pecani, Kresti³; Jeong, Jooyeon¹; Anderson, Cheyenne¹; Chen, Chen⁴; Berry, Jeffrey¹; Xia, Ming¹; Tzeng, Shin-Cheng¹ ; Becker, Eric¹; Pazouki, Leila¹; Evans, Bradley¹; Cross, Fred³; Cheng, Jianlin⁴; Czymmek, Kirk¹ ; Schröda, Michael⁵ ; Mühlhaus, Timo² ; Zhang, Ru¹ 

Show affiliations

Style APA

1
Citation

Zhang, N., Mattoon, E., McHargue, W., Venn, B., Zimmer, D., Pecani, K., Jeong, J., Anderson, C., Chen, C., Berry, J., Xia, M., Tzeng, S.-C., Becker, E., Pazouki, L., Evans, B., Cross, F., Cheng, J., Czymmek, K., Schröda, M., ... Zhang, R. (2023). Systems-wide investigation of responses to moderate and acute high temperatures in the green alga Chlamydomonas reinhardtii. [Data set]. DataPLANT. <https://doi.org/10.60534/9e5jx-75d83>

Description

hosted on: <https://git.nfd4plants.org/projects/122>

Files

arc-summary.md

[Data set] Systems-wide investigation of responses to moderate and acute high temperatures in the green alga Chlamydomonas reinhardtii.

File contents:

- root
 - isa.investigation.xlsx
 - README.md
 - runs

2

 Edit

 New version

 Share

Versions

Version v1	Sep 7, 2023
10.60534/9e5jx-75d83	

Details

DOI

DOI [10.60534/9e5jx-75d83](https://doi.org/10.60534/9e5jx-75d83)

Resource type

Dataset

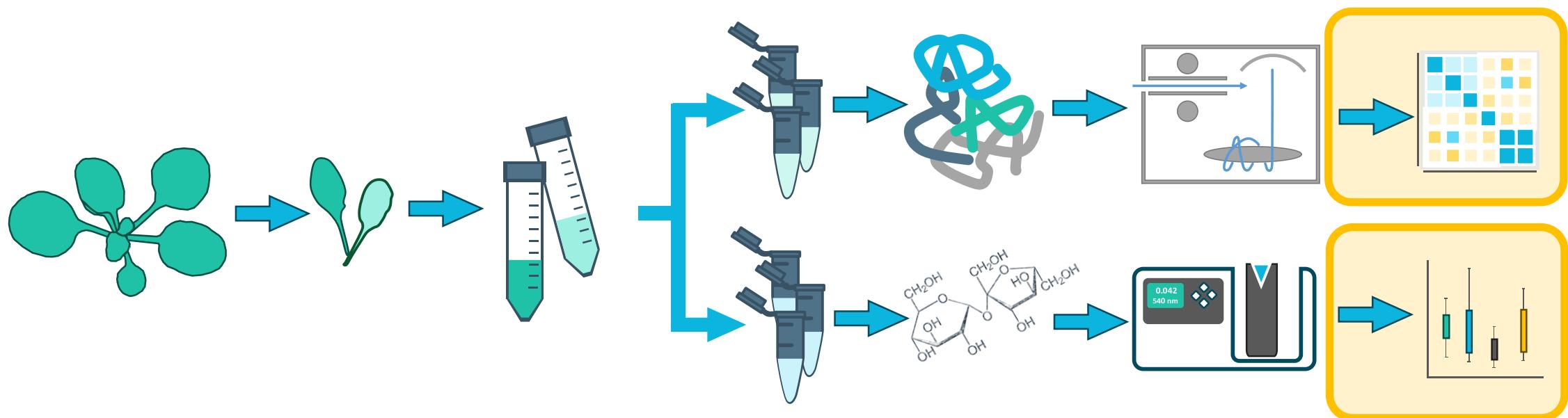
Publisher

DataPLANT

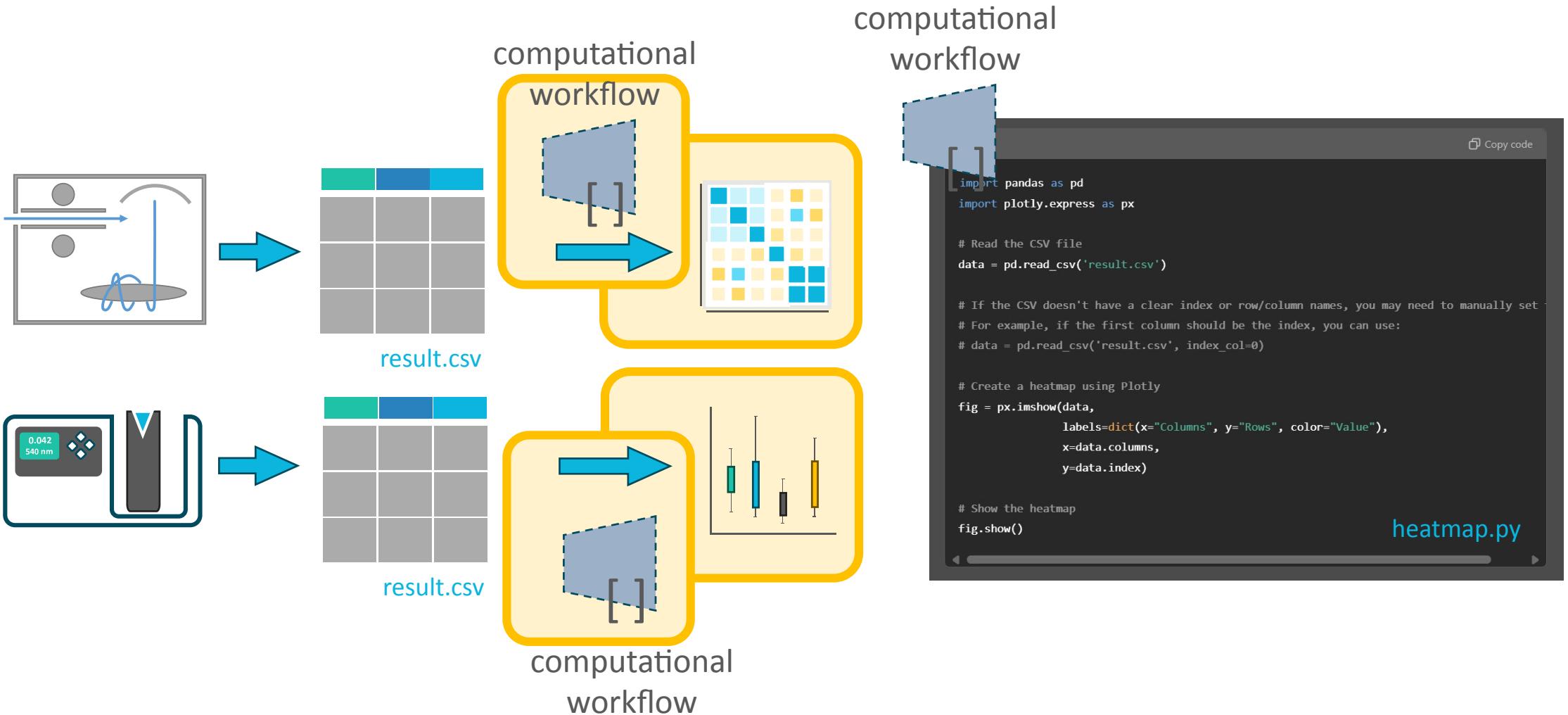
Export

JSON 

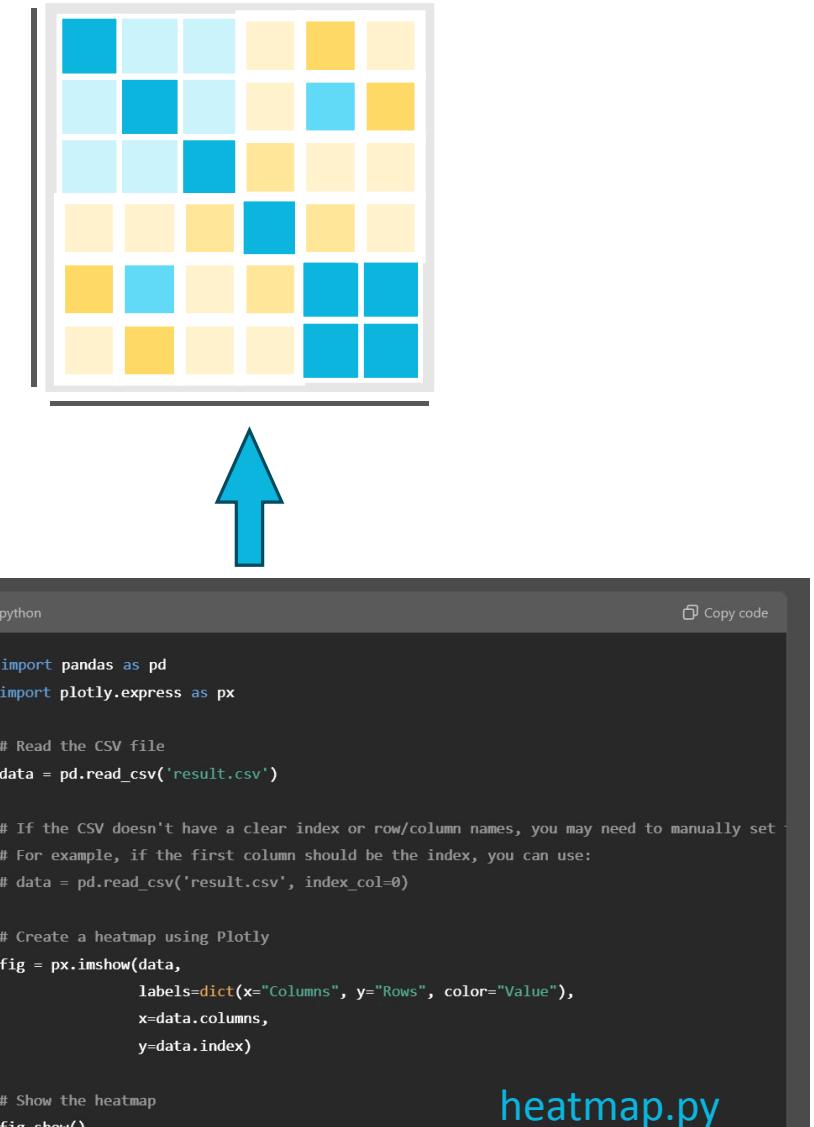
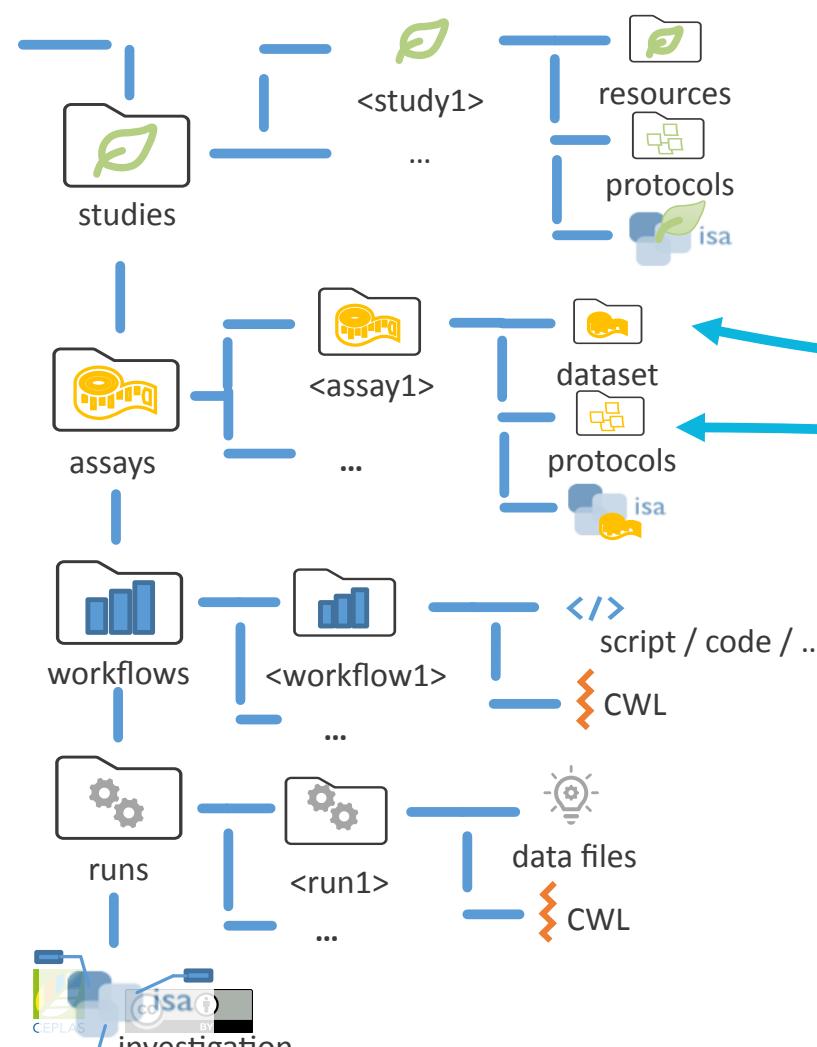
Options to annotate the data analysis



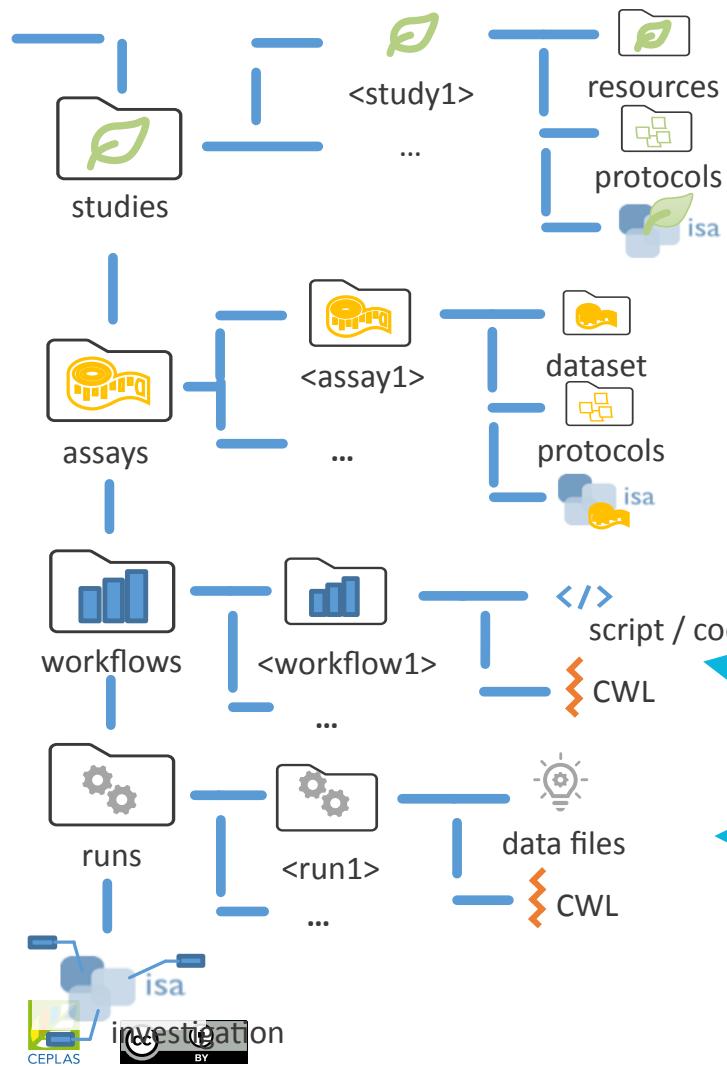
A computational workflow is like a protocol



Option I: Create a virtual assay



Option II: Create a workflow and run



```
python
Copy code

import pandas as pd
import plotly.express as px

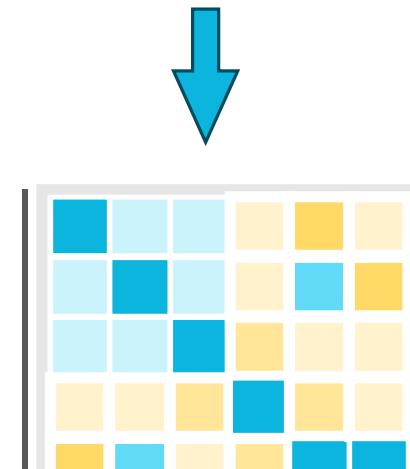
# Read the CSV file
data = pd.read_csv('result.csv')

# If the CSV doesn't have a clear index or row/column names, you may need to manually set
# For example, if the first column should be the index, you can use:
# data = pd.read_csv('result.csv', index_col=0)

# Create a heatmap using Plotly
fig = px.imshow(data,
                 labels=dict(x="Columns", y="Rows", color="Value"),
                 x=data.columns,
                 y=data.index)

# Show the heatmap
fig.show()
```

heatmap.py



Use CWL to wrap your workflow

CWL workflow document (*.cwl)

```
graph LR; A[1] --> B(( )); B --> C[3];
```

```
#!/usr/bin/env cwl-runner

cwlVersion: v1.0
class: Workflow
inputs:
  tarball: File
  name_of_file_to_extract: string

outputs:
  compiled_class:
    type: File
    outputSource: compile/classfile

steps:
  untar:
    run: tar-param.cwl
    in:
      tarfile: tarball
      extractfile: name_of_file_to_extract
    out: [extracted_file]

    compile:
      run: arguments.cwl
      in:
        src: untar/extracted_file
      out: [classfile]
```

CWL
tool descriptors (*.cwl)

CWL job parameter (*.yaml)

```
job
yaml

file: fastq
param: 5
workflow: wf.cwl
output_folder:
  /temp
```

CWL runner



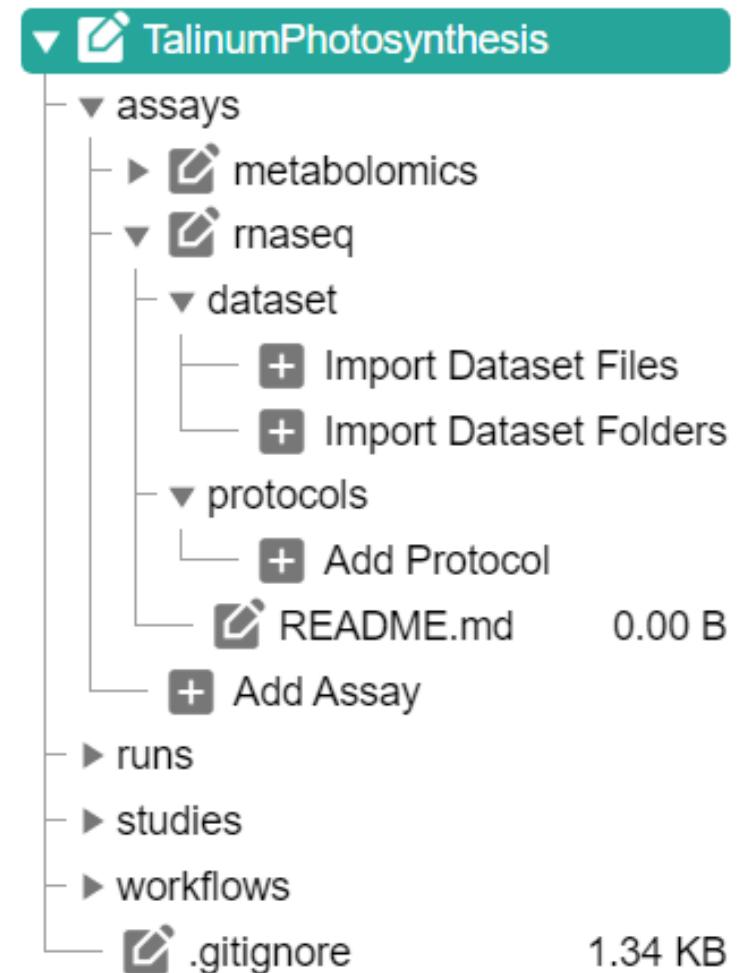
Add datasets

In the file tree you can

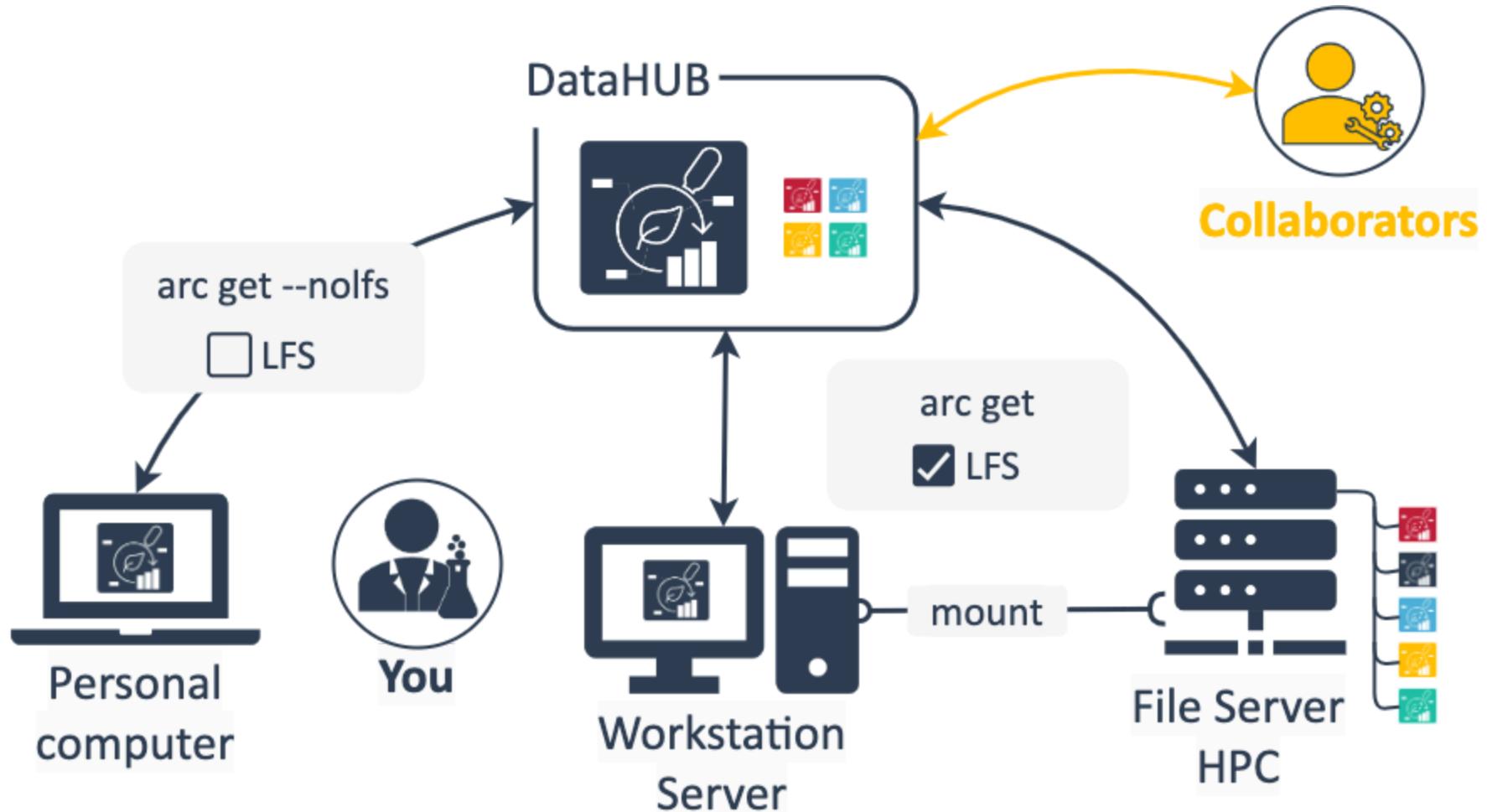
- **import dataset files or folders** and
- **protocols** associated to that dataset.

 **Import Dataset** allows to import data from any location on your computer into the ARC.

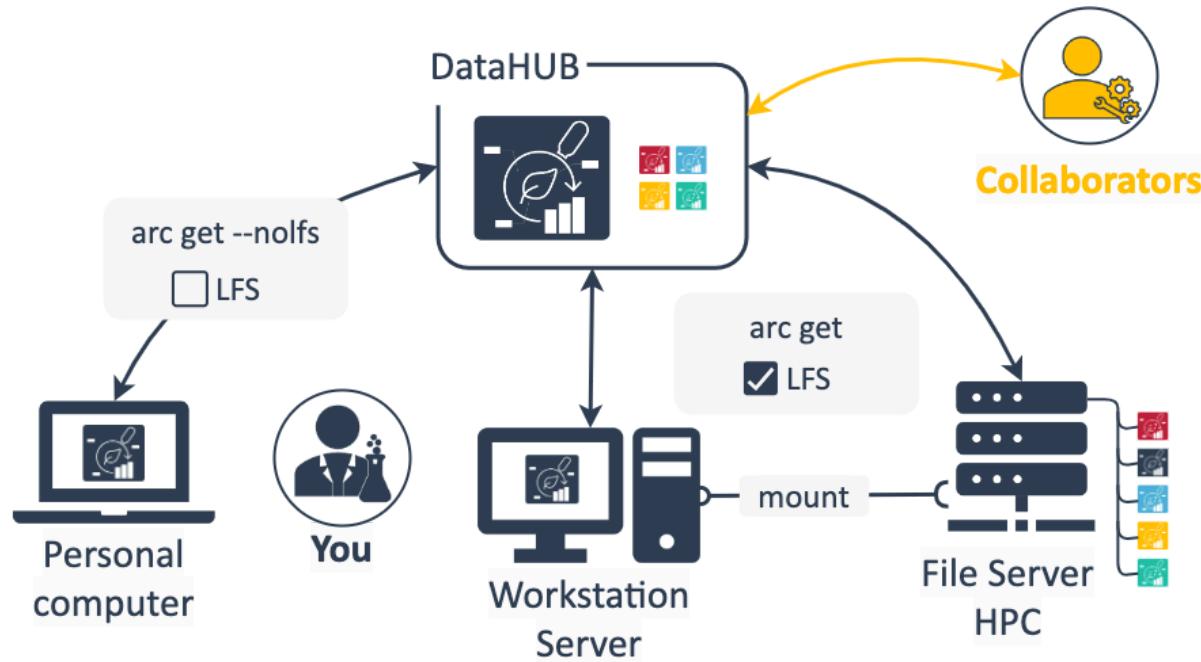
 Depending on the file size, this may take a while. Test this with a small batch of files first.



Where do I store my ARC?



ARC storage and sharing



- DataHUB as "ground truth" / original clone
- You can sync and communicate all changes to your ARC via the DataHUB

💡 ARCitect and ARC commander provide options to avoid syncing large files (LFS = Large file storage)

Example setup to store and use ARCs

Personal computer

- work on small files
- annotate metadata
- add scripts, protocols

Workstation / Server

- work on large files
- run computations

FileShare

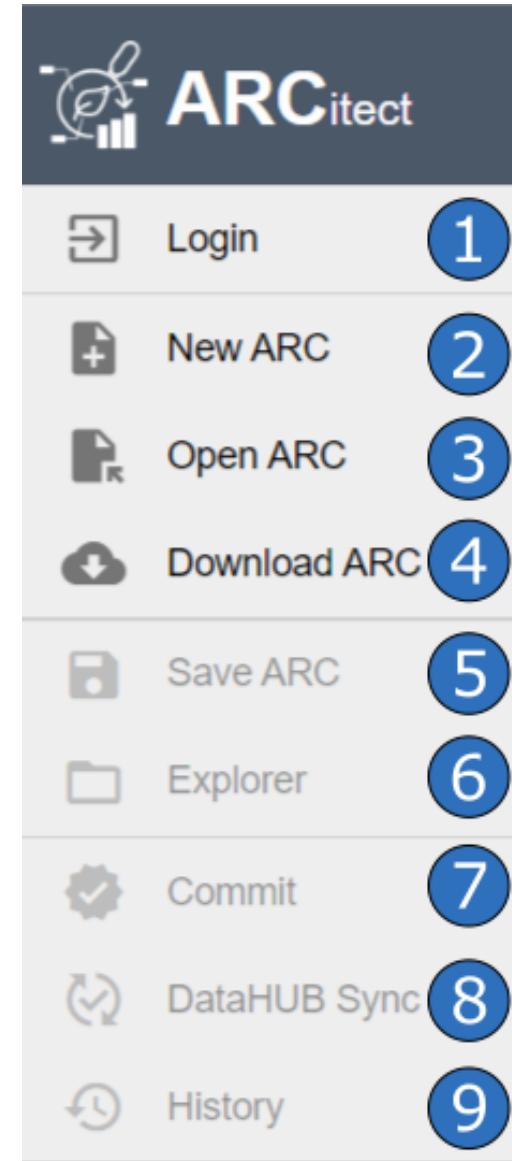
- mount to local machine, sync ARC from there

HPC

- direct connection HPC to DataHUB (depends on security settings)
- or mount to local machine and sync, ARC from there

Download the demo data

1. Open the ARCitect
2. Login (1) to your DataHUB account
3. Navigate to Download ARC (4)

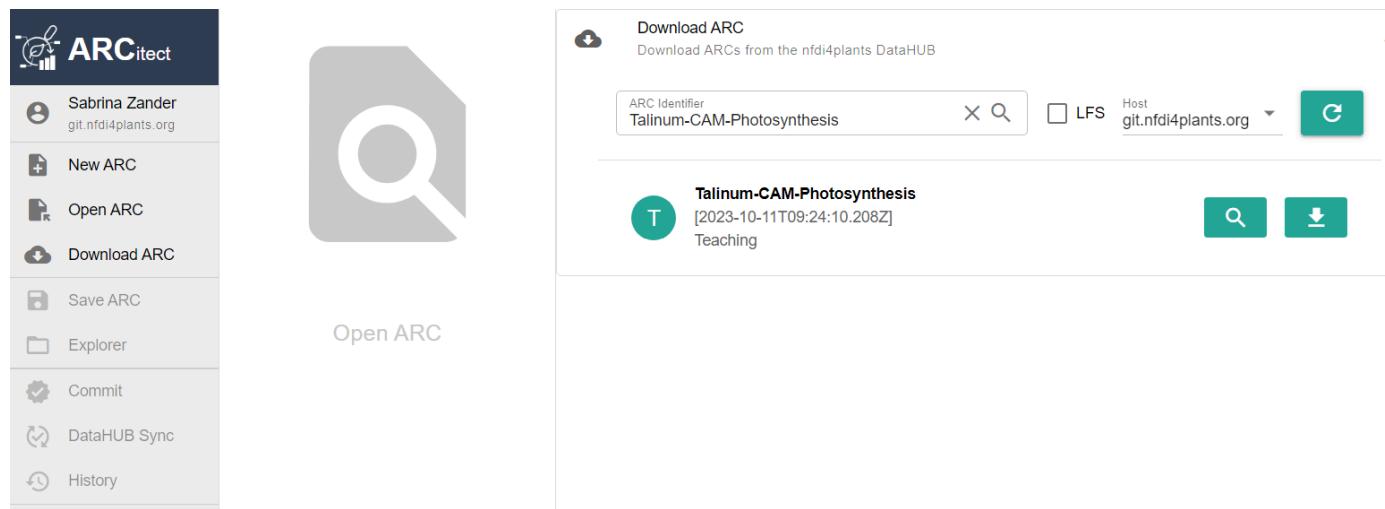


Download the demo data

4. Search for **Talinum-CAM-Photosynthesis**

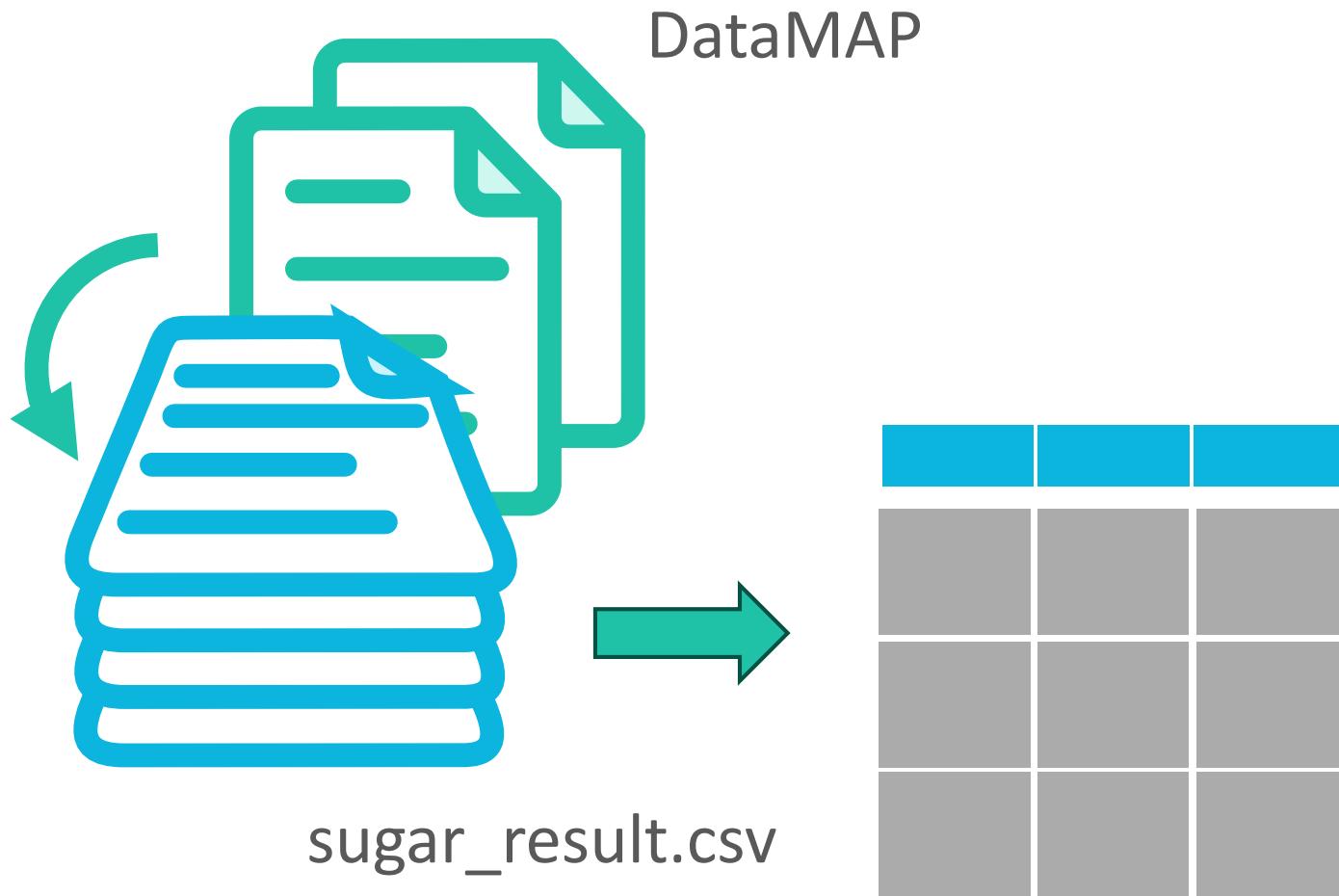
5. Click the download button, select a location and open the ARC.

6. Open the downloaded ARC

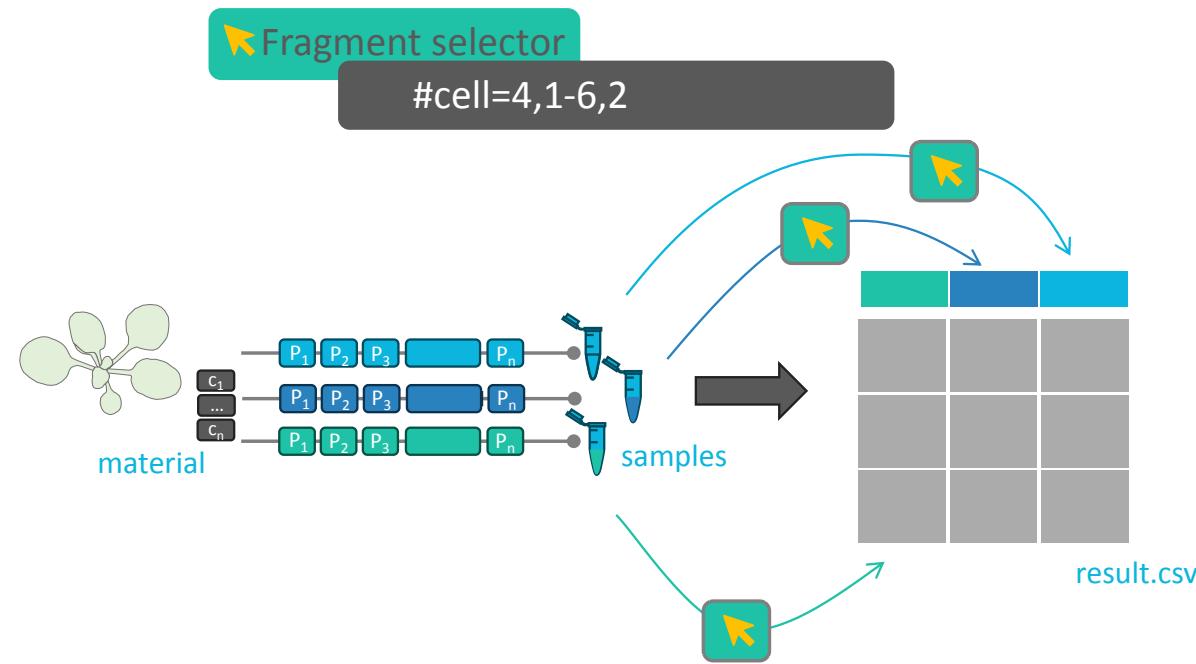


 This is basically the ARC we created in the last session.

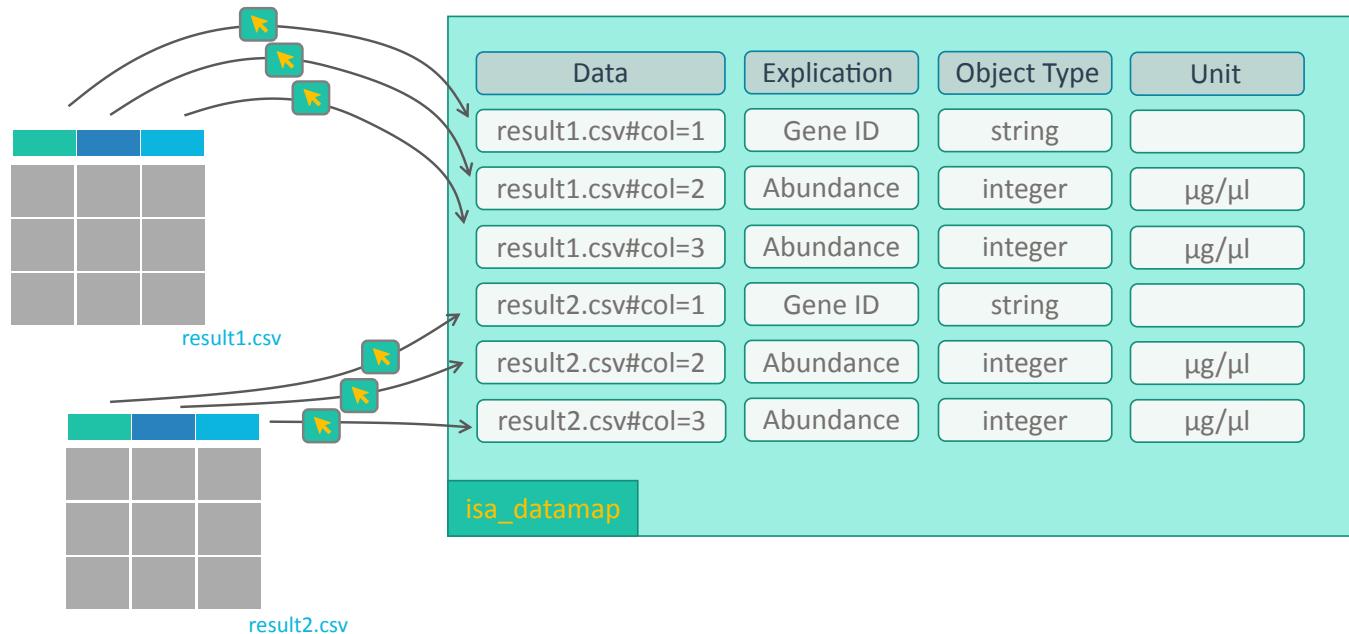
Annotation of the result data points



Point into results - Fragment selectors



DataMAP: Annotation for the fragment selectors



Contributors

If not referenced otherwise, figures and slides presented here were created by members of DataPLANT (<https://nfdi4plants.org>).

Additional slides were contributed by

- name: Dominik Brilhaus
github: <https://github.com;brilator>
orcid: <https://orcid.org/0000-0001-9021-3197>
- name: Cristina Martins Rodrigues
github: <https://github.com/CMR248>
orcid: <https://orcid.org/0000-0002-4849-1537>
- name: Kevin Frey
github: <https://github.com/Freymaurer>
orcid: <https://orcid.org/0000-0002-8493-1077>
- name: Sabrina Zander
orcid: <https://orcid.org/0009-0000-4569-6126>
- name: Martin Kuhl
github: <https://github.com/Martin-Kuhl>
orcid: <https://orcid.org/0000-0002-8493-1077>

