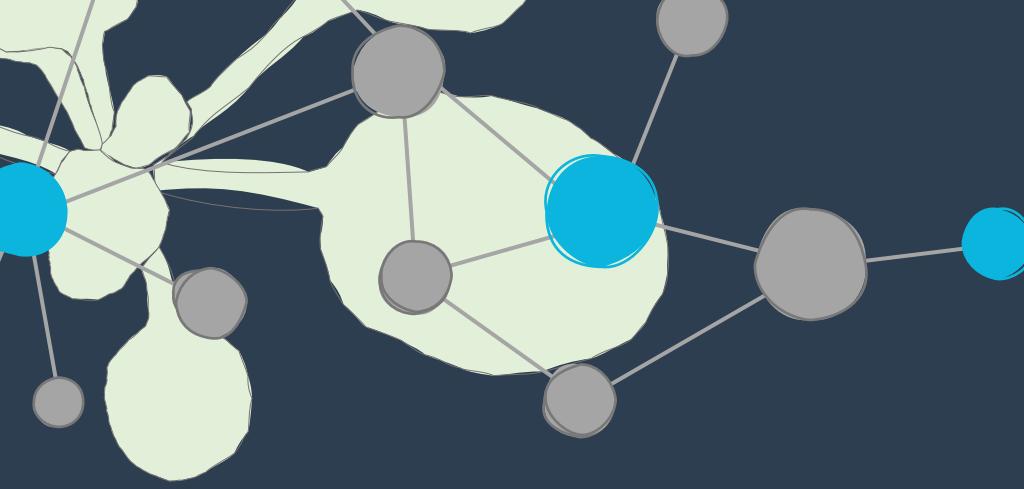
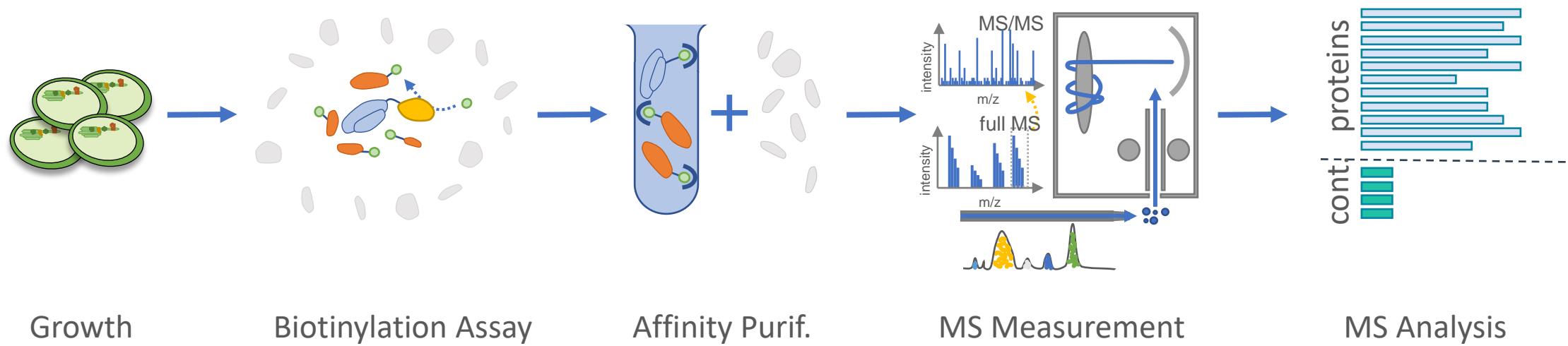


Becoming FAIR: Utilizing ARCs and the PLANTdataHUB for collaborative research in the TRR175



Part two: What is an ARC? A Practical Approach

Motivation: An TurboID experiment

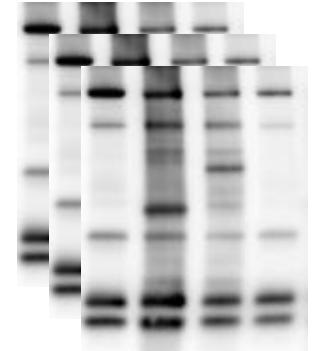
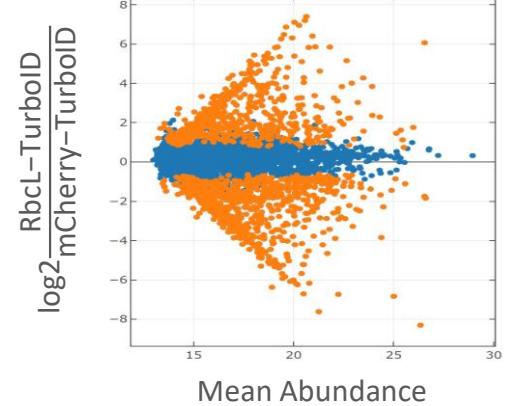
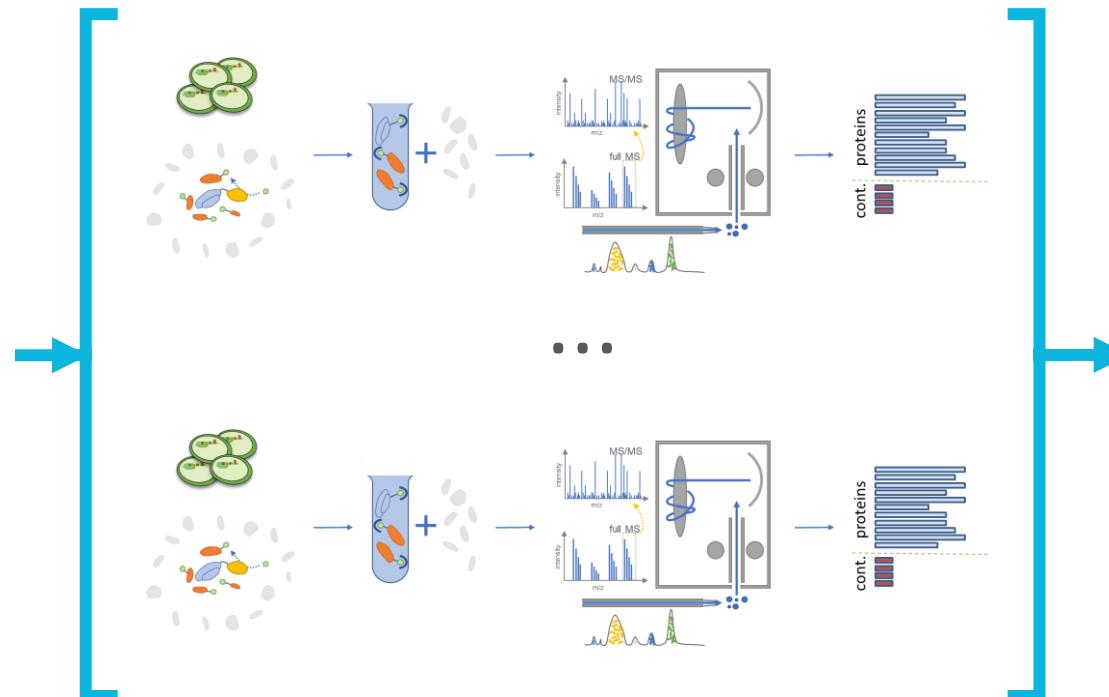


Motivation: An TurbolD experiment

Cell type 1,
genetic background 1,
Condition 1
e.g. RbcL-TurbolD

...

Cell type n,
genetic background n,
Condition n
e.g. mCherry-TurbolD

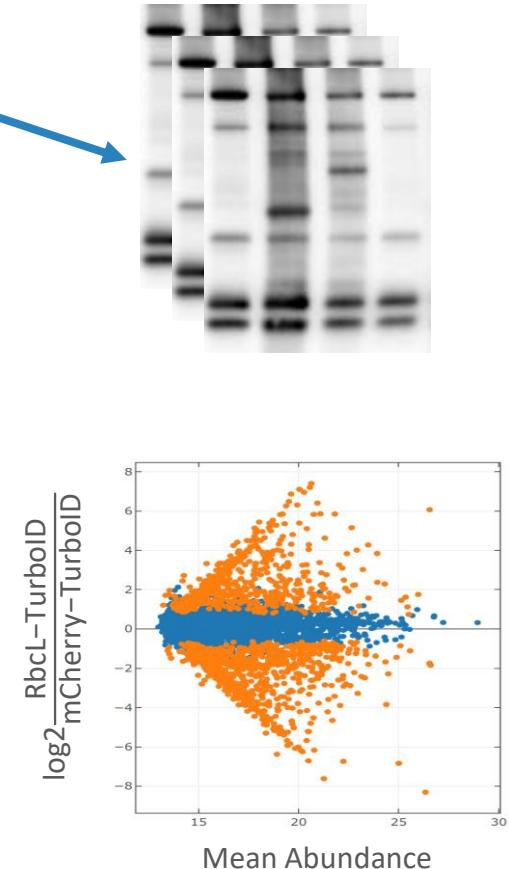
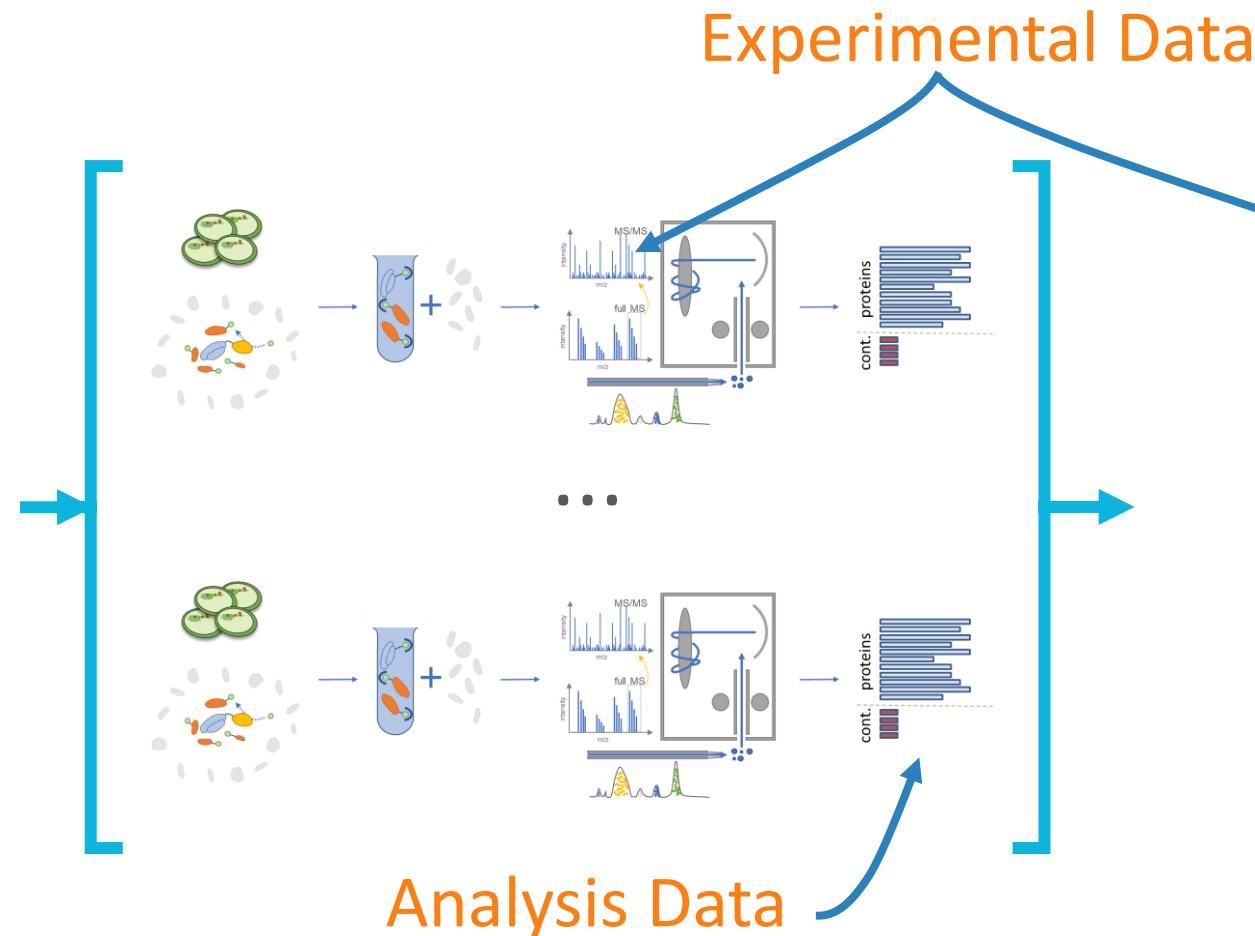


Motivation: An TurboID experiment

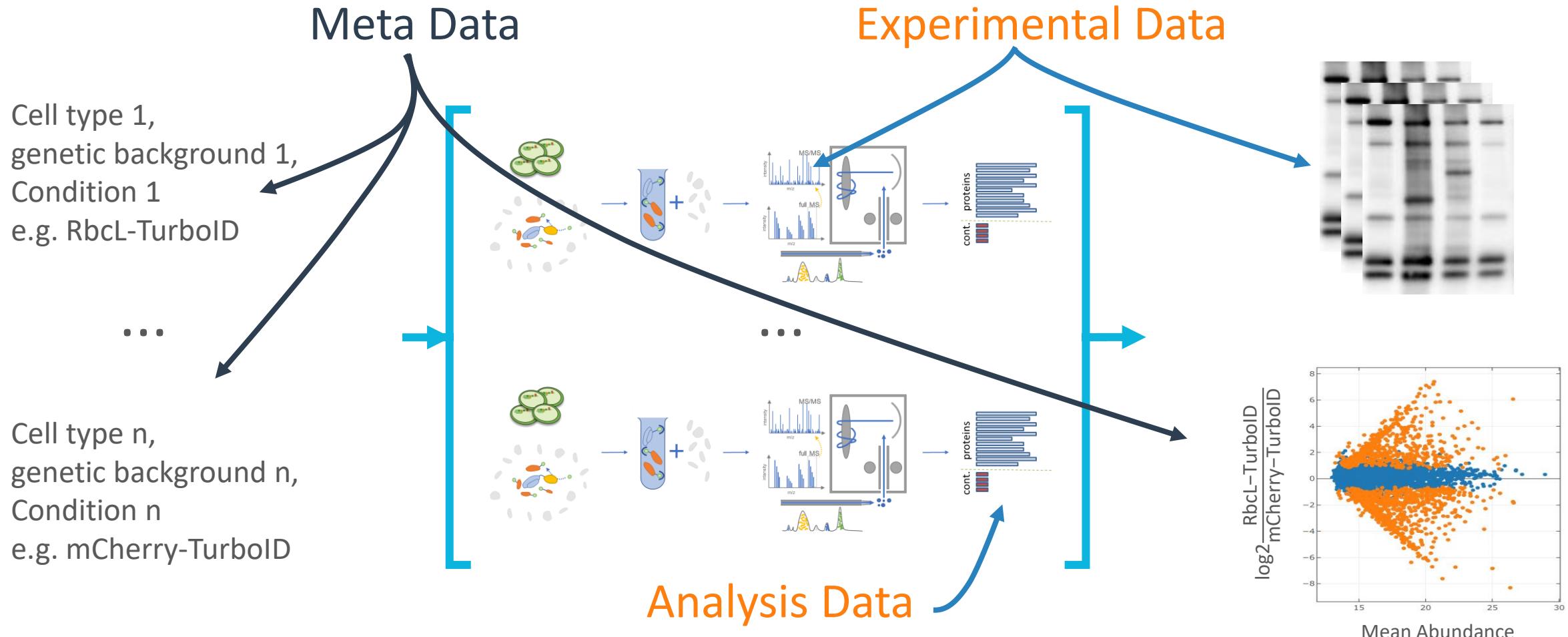
Cell type 1,
genetic background 1,
Condition 1
e.g. RbcL-TurboID

...

Cell type n,
genetic background n,
Condition n
e.g. mCherry-TurboID

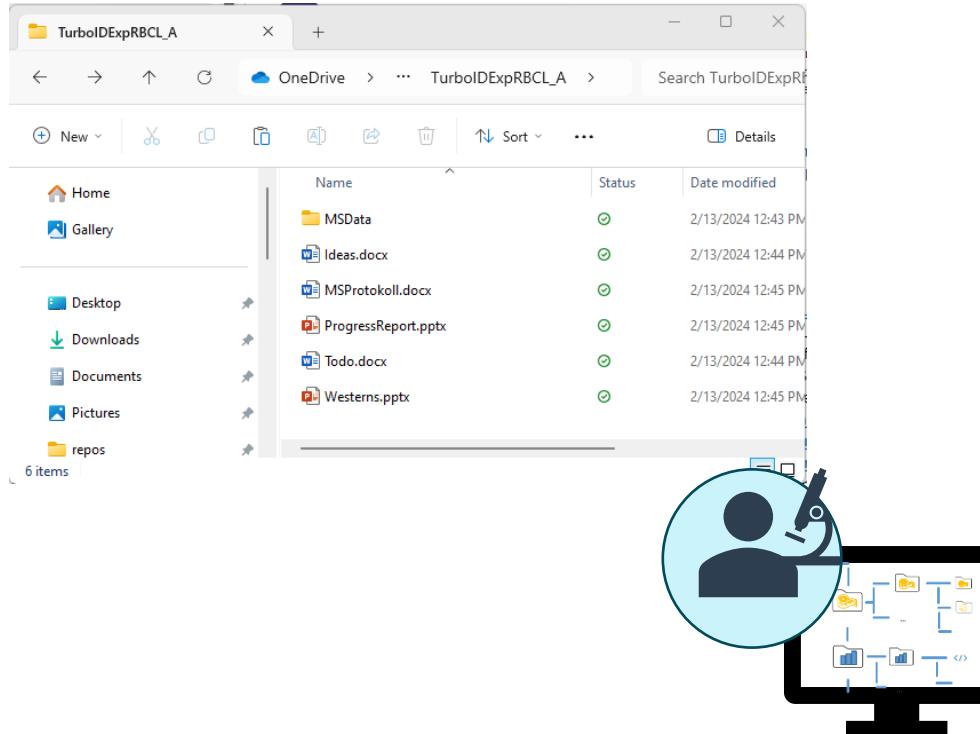


Motivation: An TurboID experiment



Until recently: Individual RDM solutions

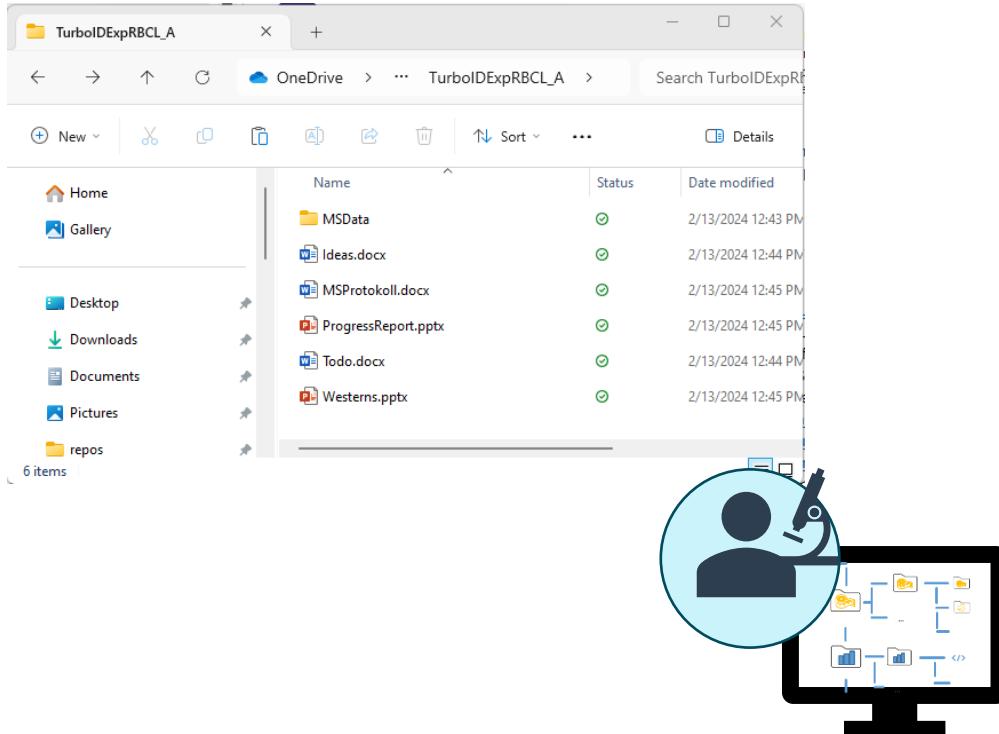
Researcher As data management solution:



Researcher A

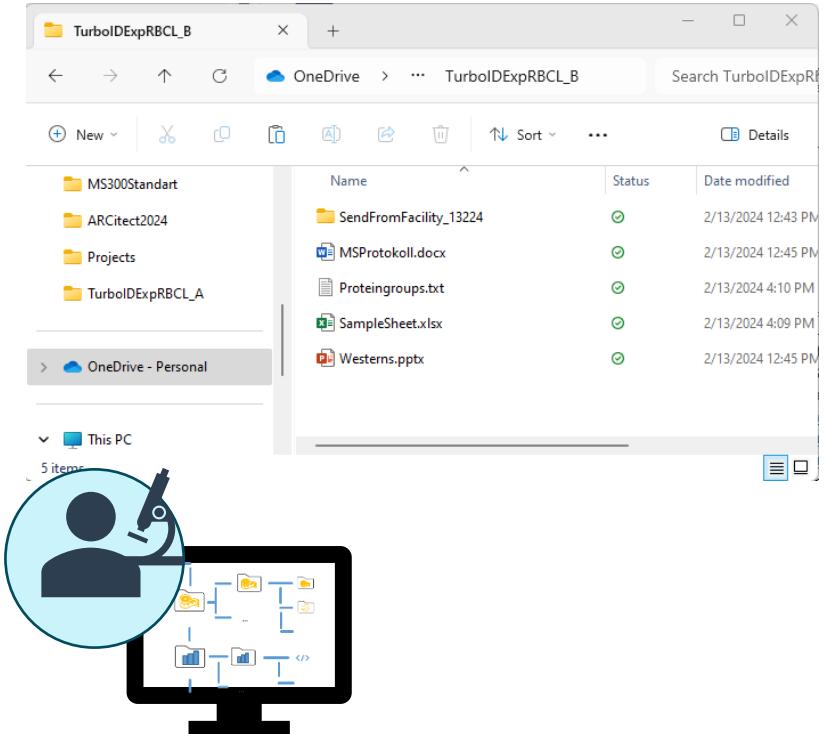
Until recently: Individual RDM solutions

Researcher As data management solution:



Researcher A

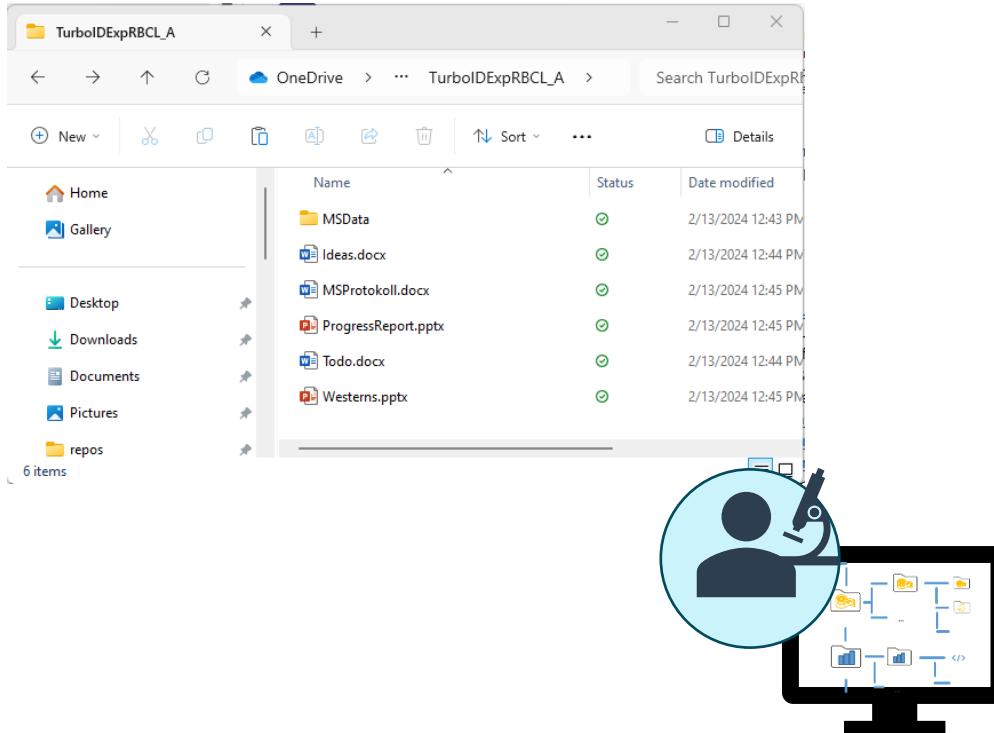
Researcher Bs data management solution:



Researcher B

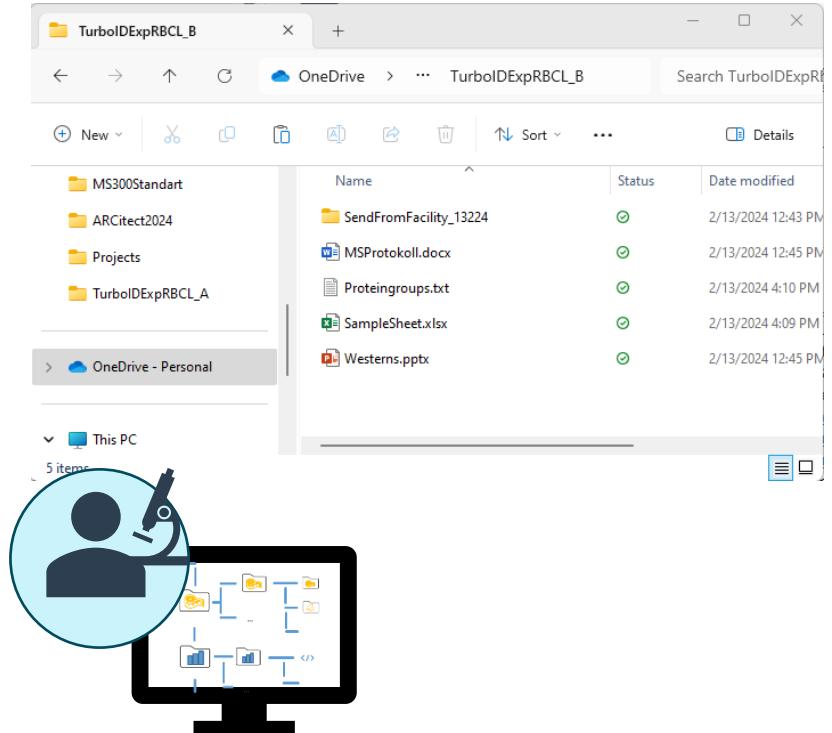
Until recently: Individual RDM solutions

Researcher As data management solution:



Researcher A

Researcher Bs data management solution:

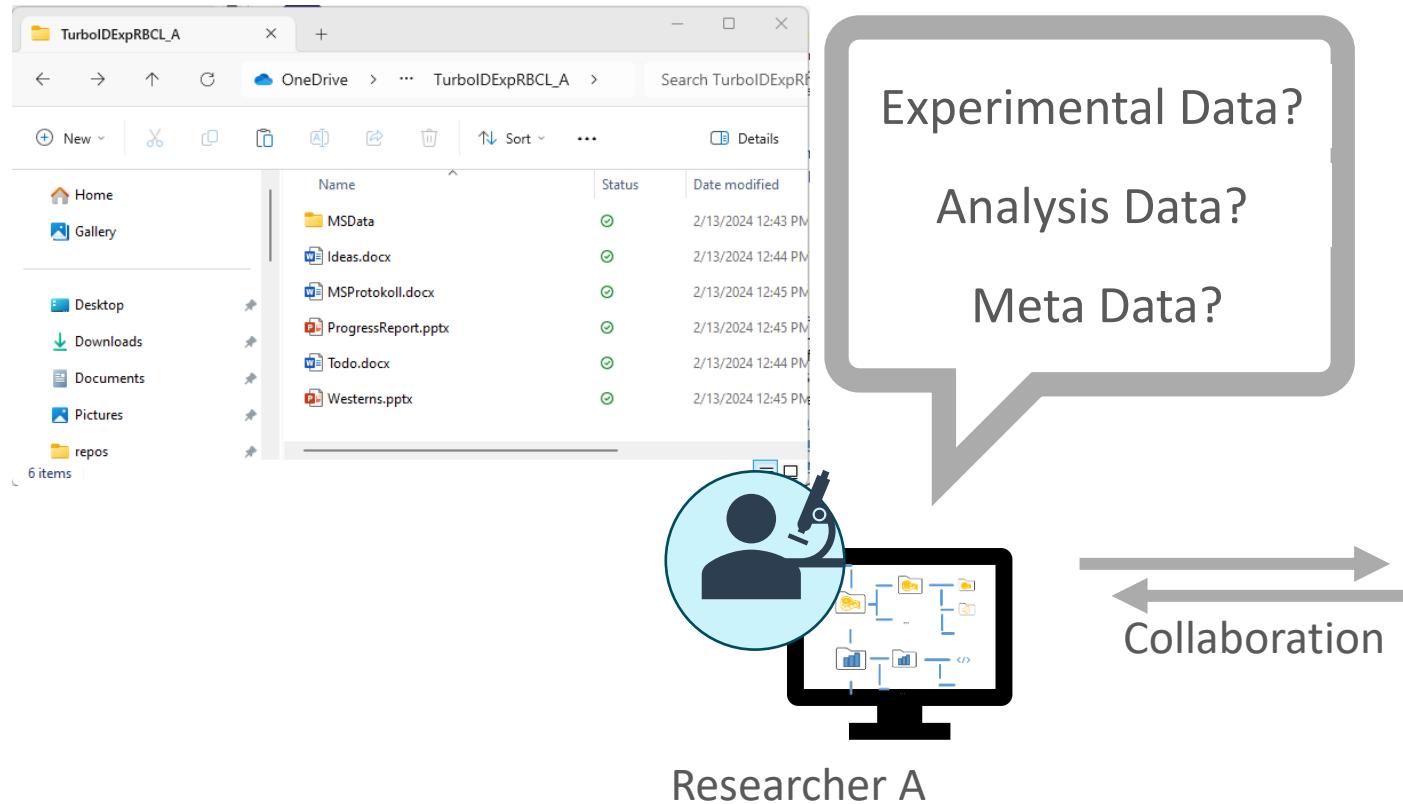


Researcher B

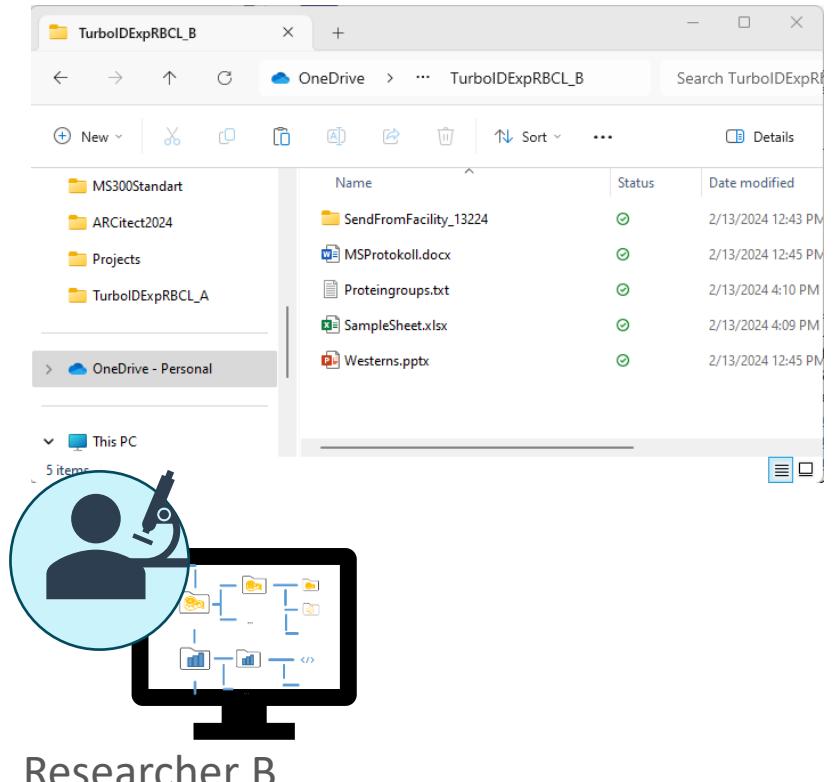
Collaboration

Until recently: Individual RDM solutions

Researcher As data management solution:

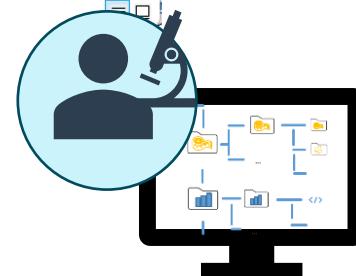
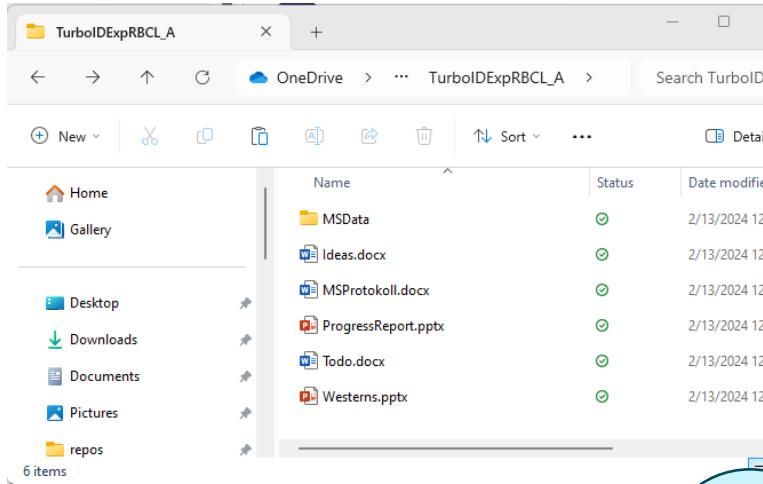


Researcher Bs data management solution:



Until recently: Individual RDM solutions

Researcher As data management solution:

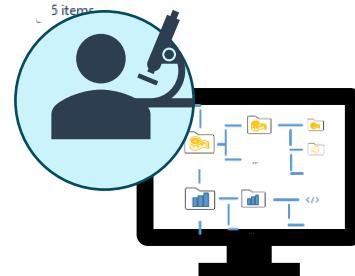
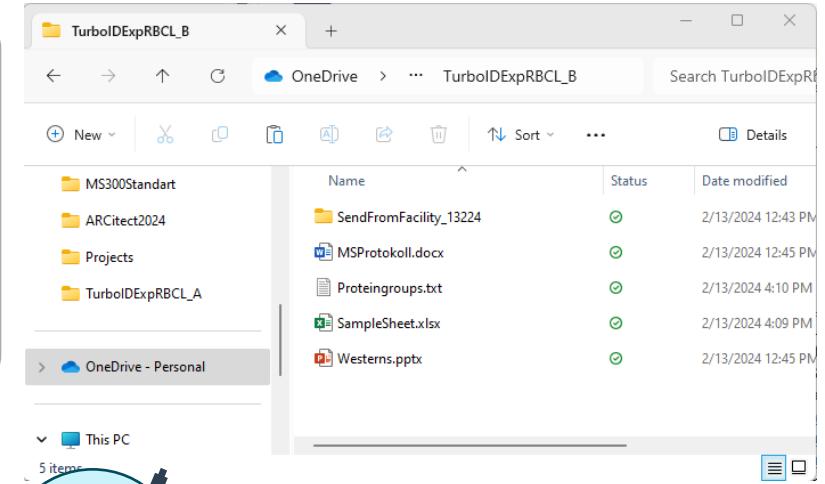


Researcher A

How do we
exchange data?
More Metadata?
Any Updates?

Collaboration

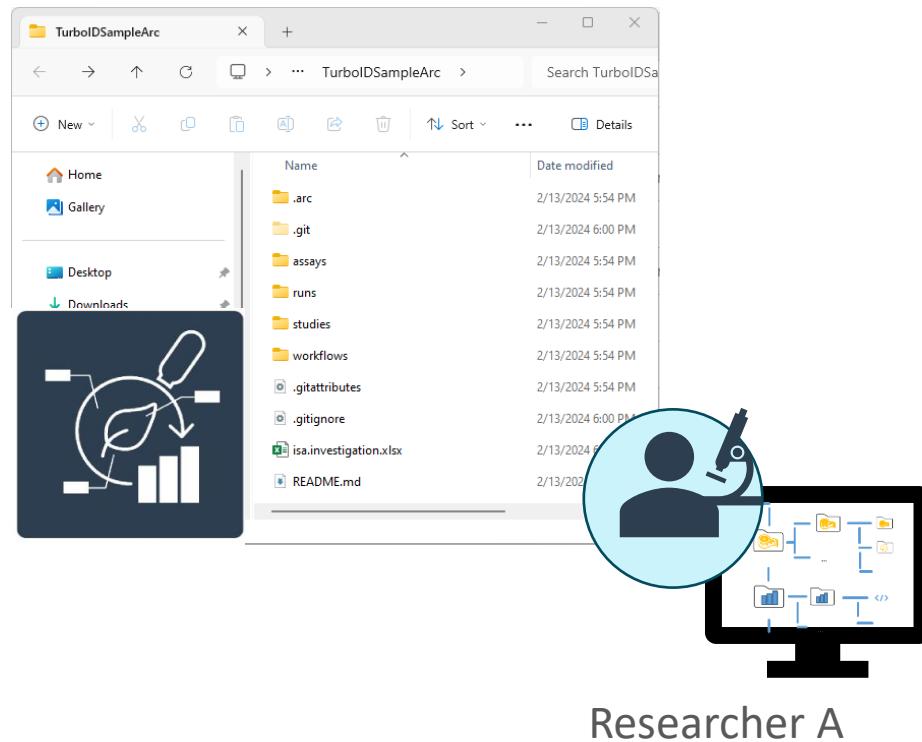
Researcher Bs data management solution:



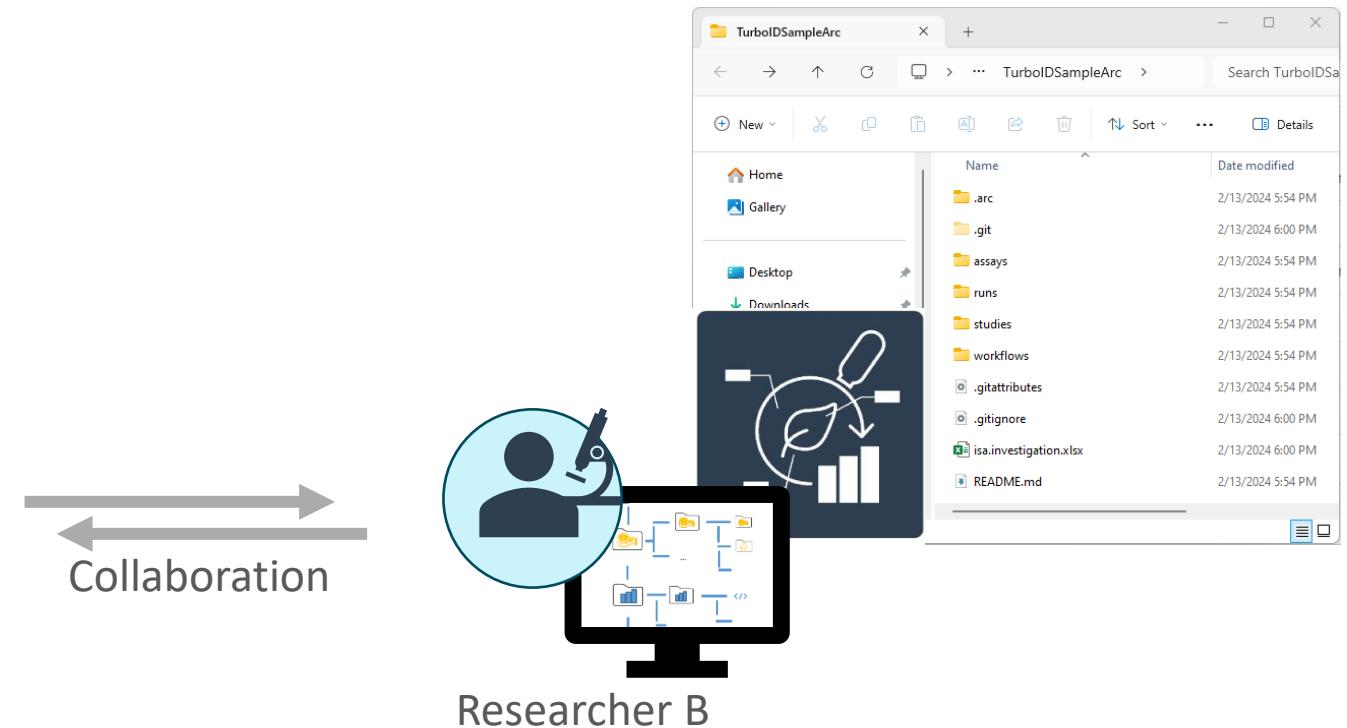
Researcher B

Now: ARCs as a single RDM entry point

Researcher As data management solution:
Annotated Research Context (ARC)



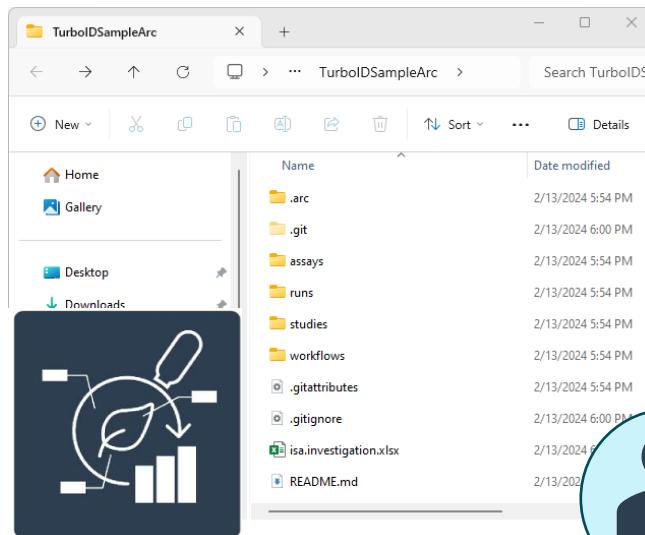
Researcher Bs data management solution:
Annotated Research Context (ARC)



Collaboration

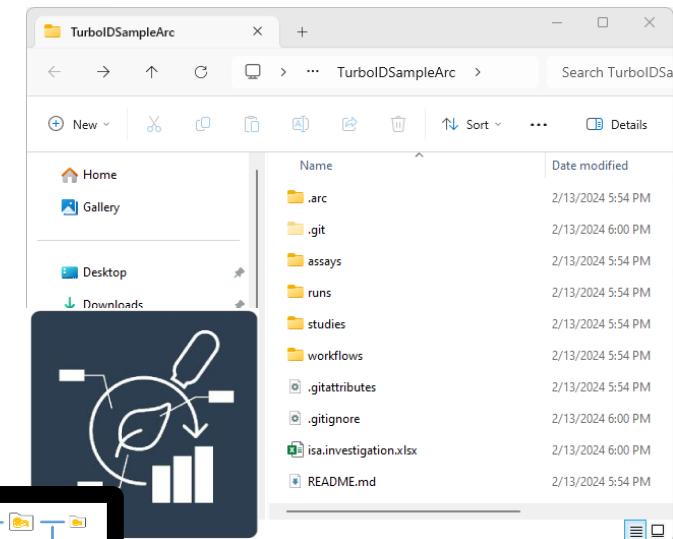
Now: ARCs as a single RDM entry point

Researcher As data management solution:
Annotated Research Context (ARC)



Researcher A

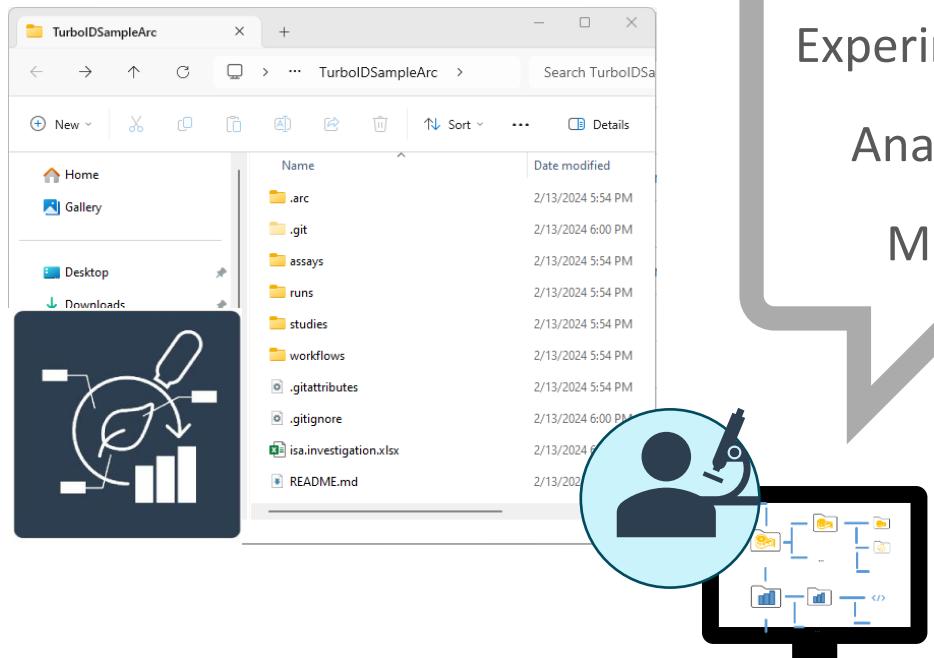
Researcher Bs data management solution:
Annotated Research Context (ARC)



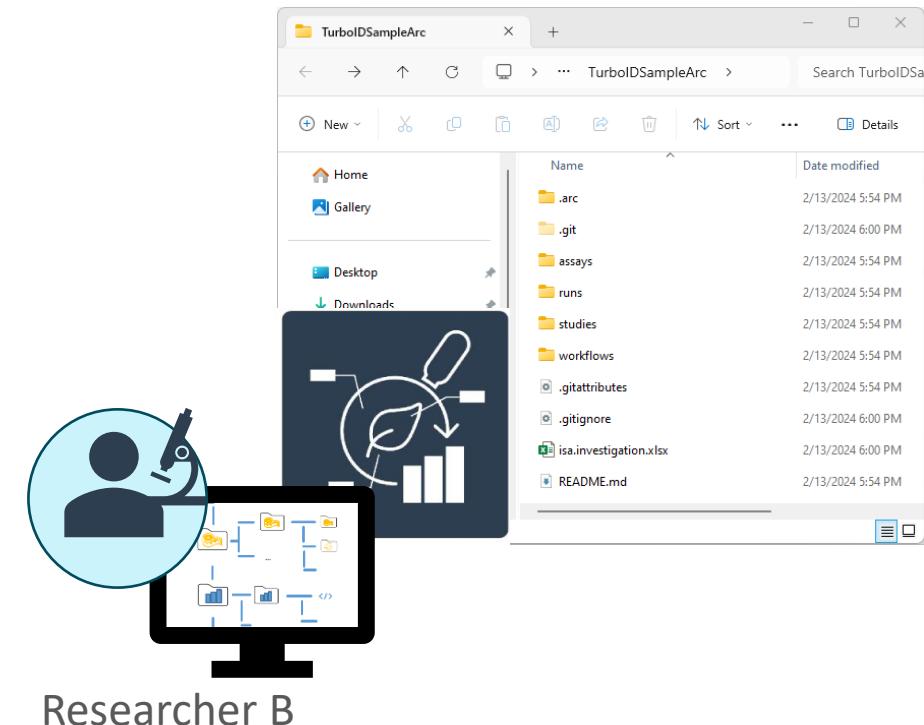
Researcher B

Now: ARCs as a single RDM entry point

Researcher As data management solution:
Annotated Research Context (ARC)

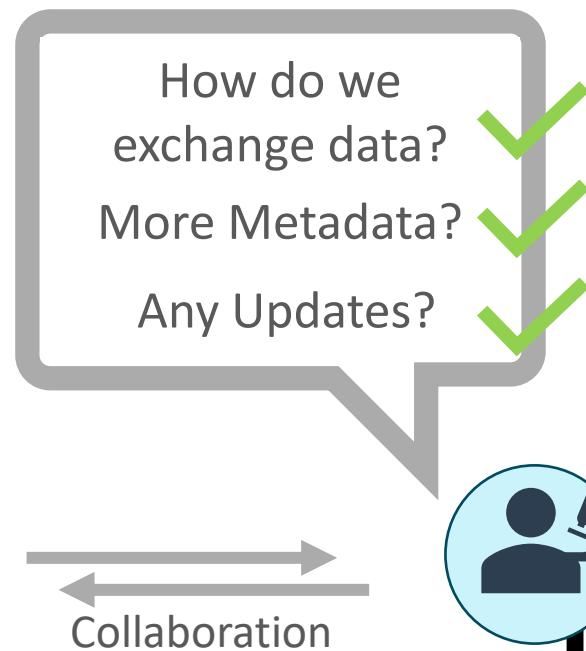
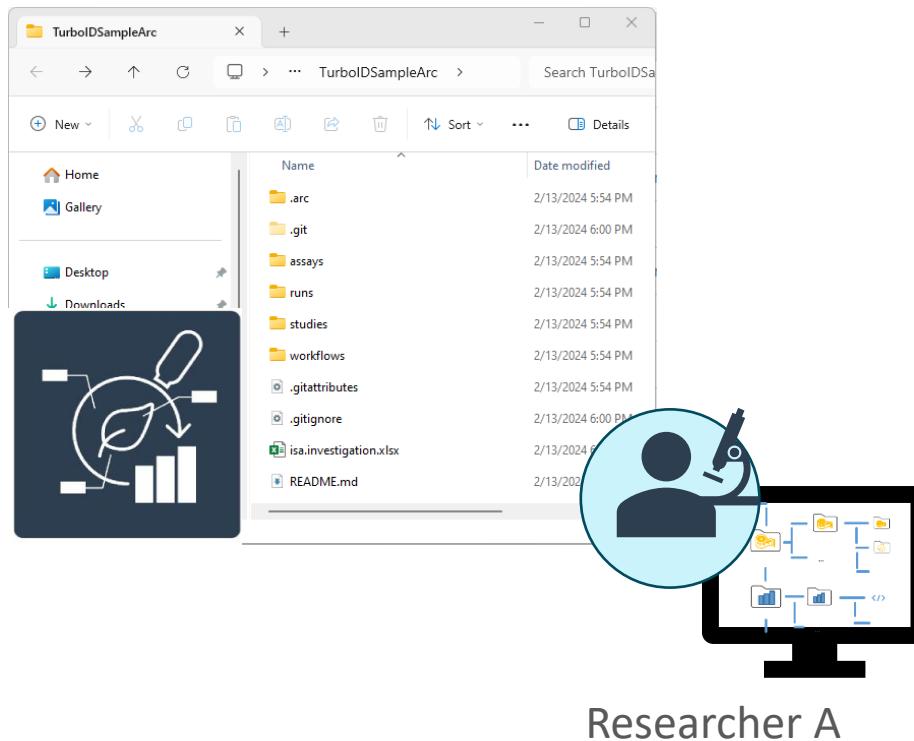


Researcher Bs data management solution:
Annotated Research Context (ARC)

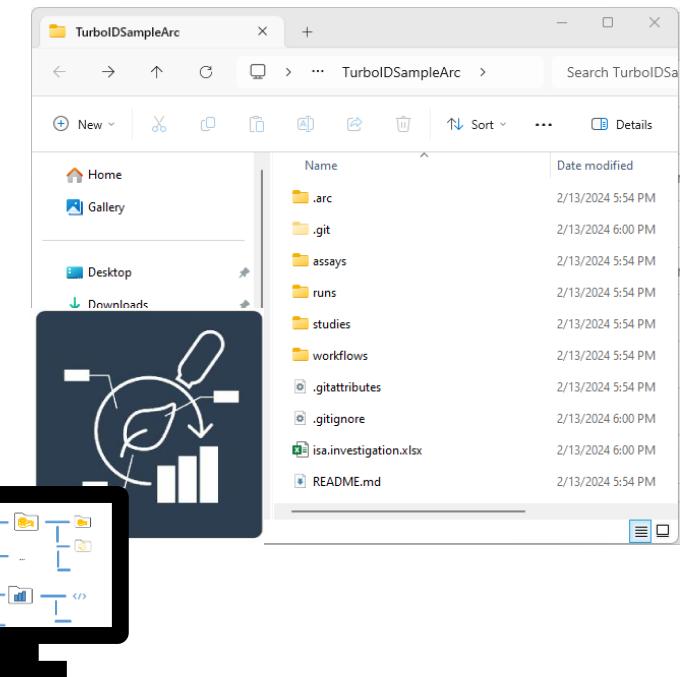


Now: Using the PLANTDataHUB to collaborate

Researcher As data management solution:
Annotated Research Context (ARC)



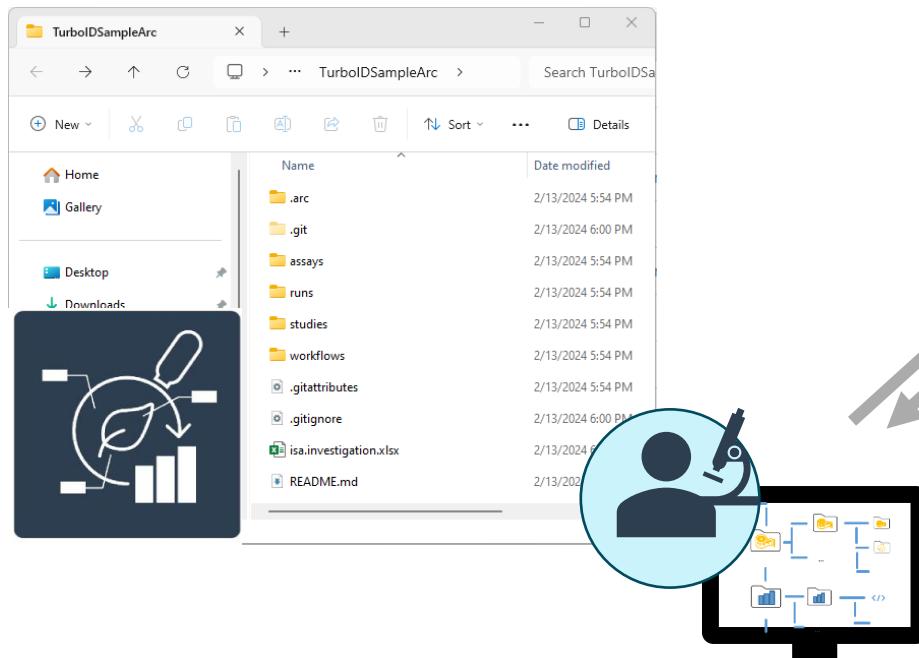
Researcher Bs data management solution:
Annotated Research Context (ARC)



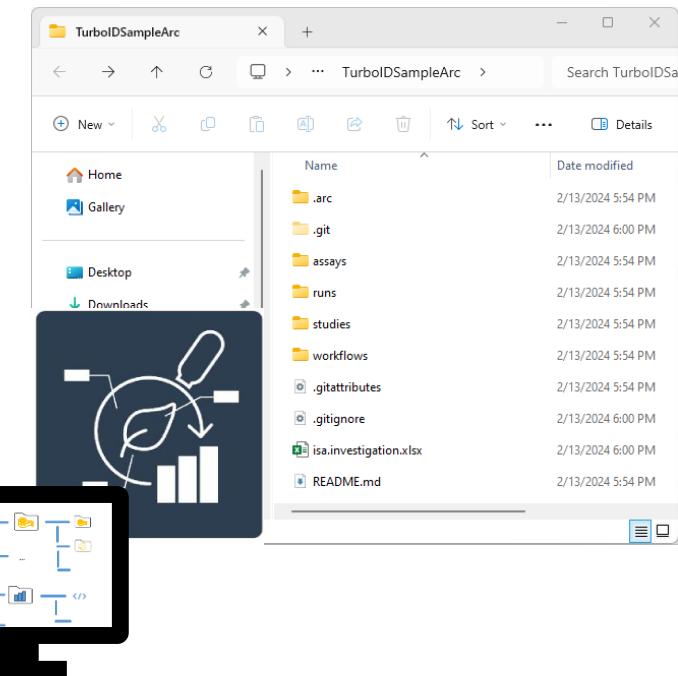
Researcher B

Now: Using the PLANTDataHUB to collaborate

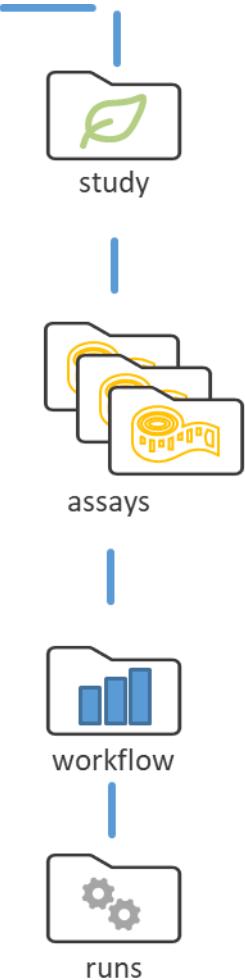
Researcher As data management solution:
Annotated Research Context (ARC)



Researcher Bs data management solution:
Annotated Research Context (ARC)



Agenda of part two



- I. Important ARC concepts by example:
Structure and Data
- II. Important ARC concepts by example:
Meta Data Annotation Principle
- III. ARCs for FAIR collaboration using the
PLANTDataHUB

IV. Complete Walk-Through
using the ARCitect



Agenda of part two

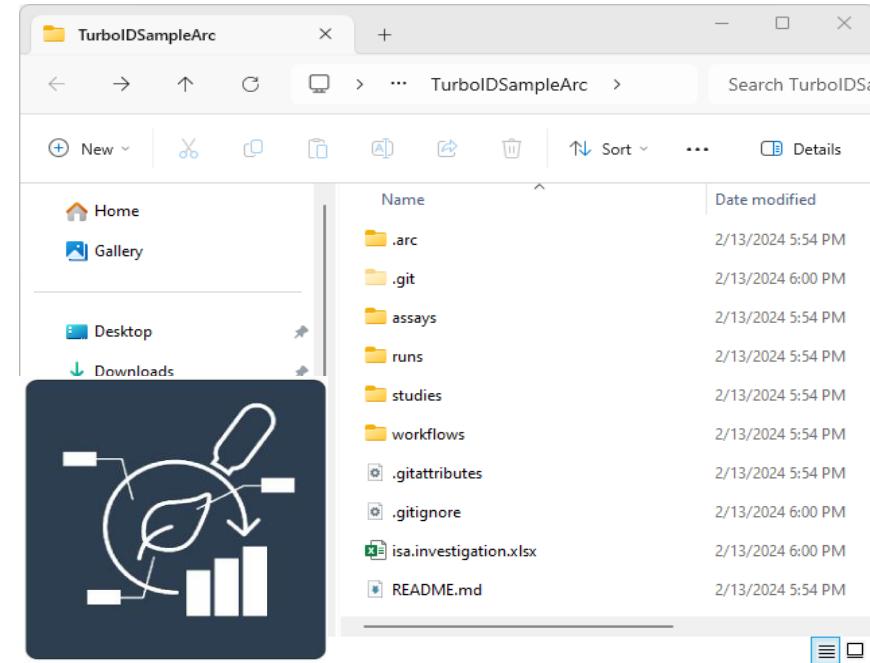
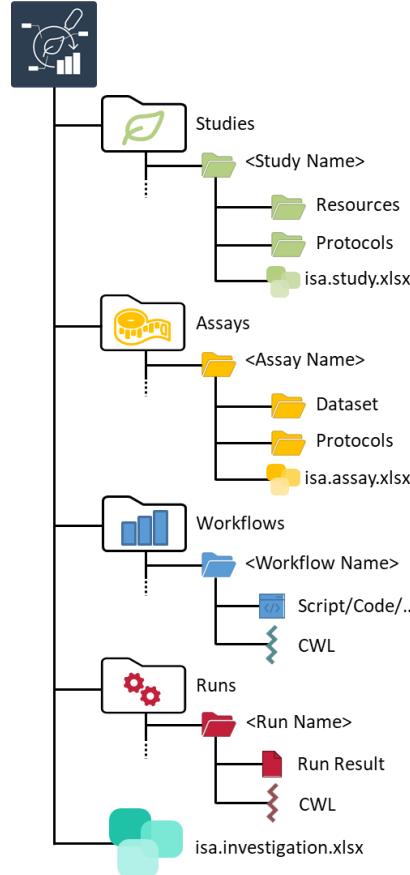


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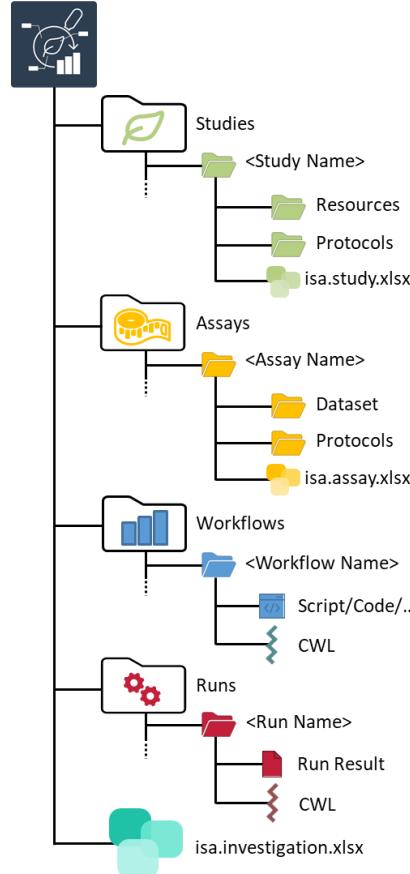
IV. Complete Walk-Through
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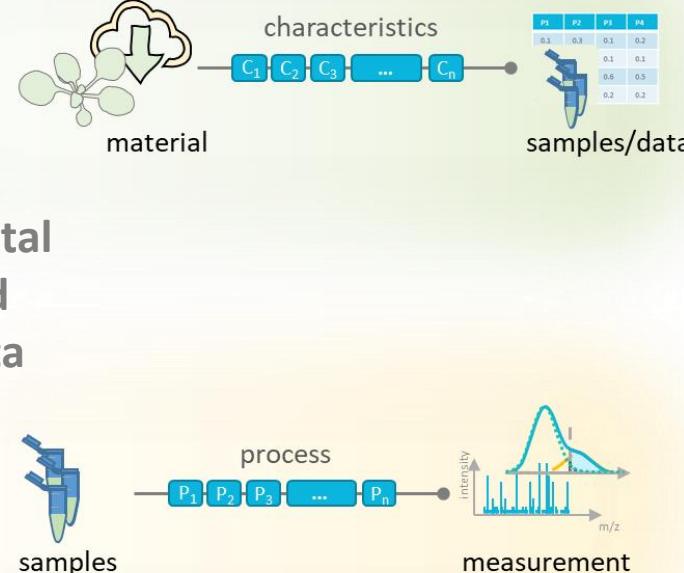
Important ARC Concepts: Structure and Data



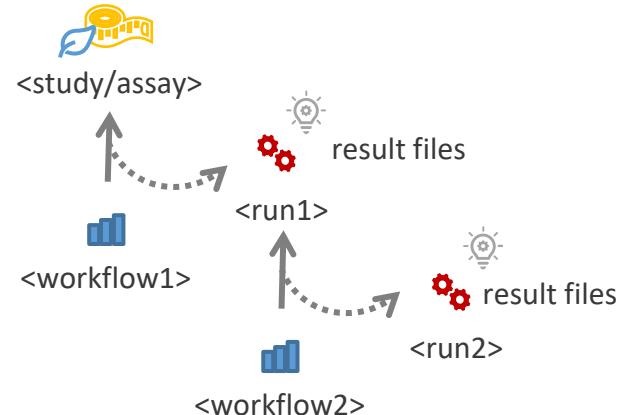
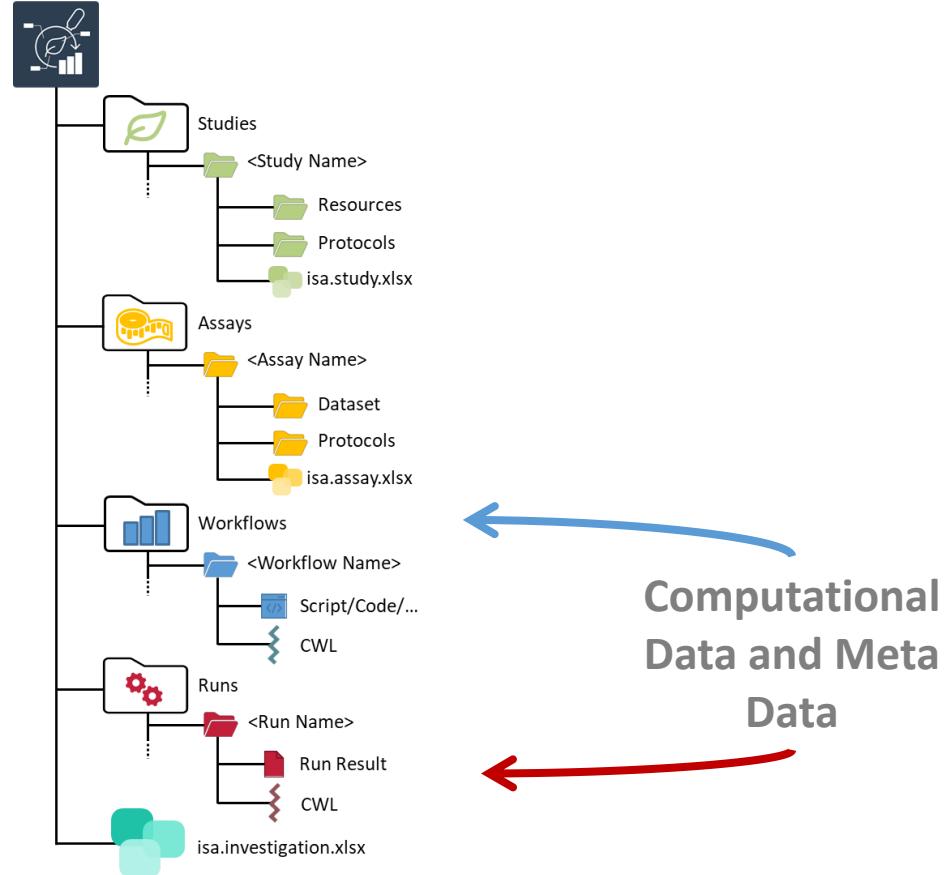
Important ARC Concepts: Structure and Data



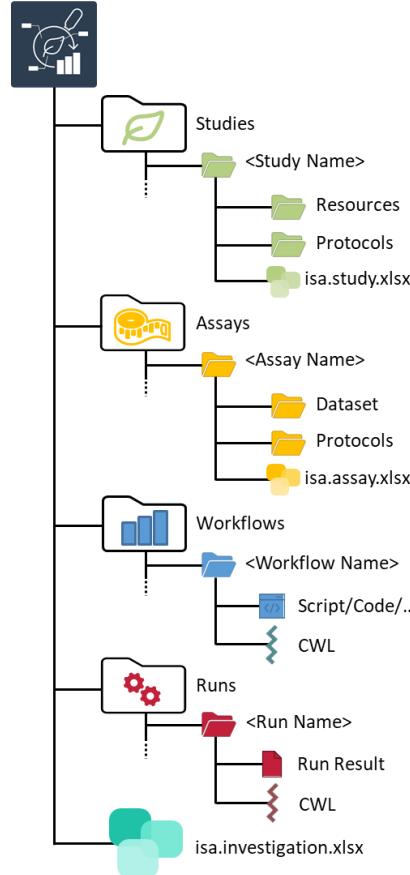
**Experimental
Data and
Meta Data**



Important ARC Concepts: Structure and Data

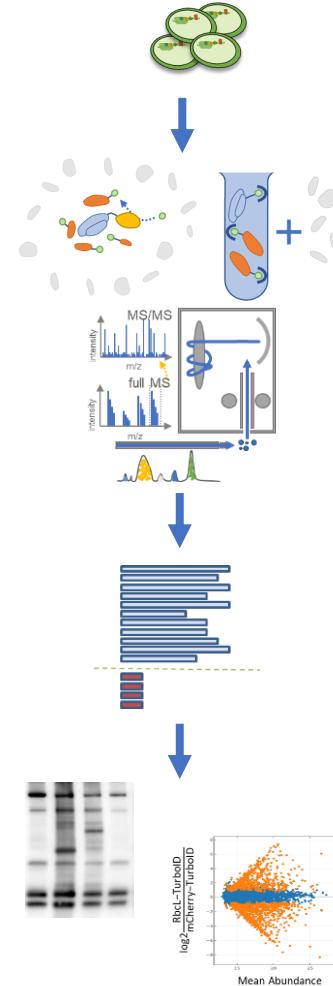


Important ARC Concepts: Structure and Data

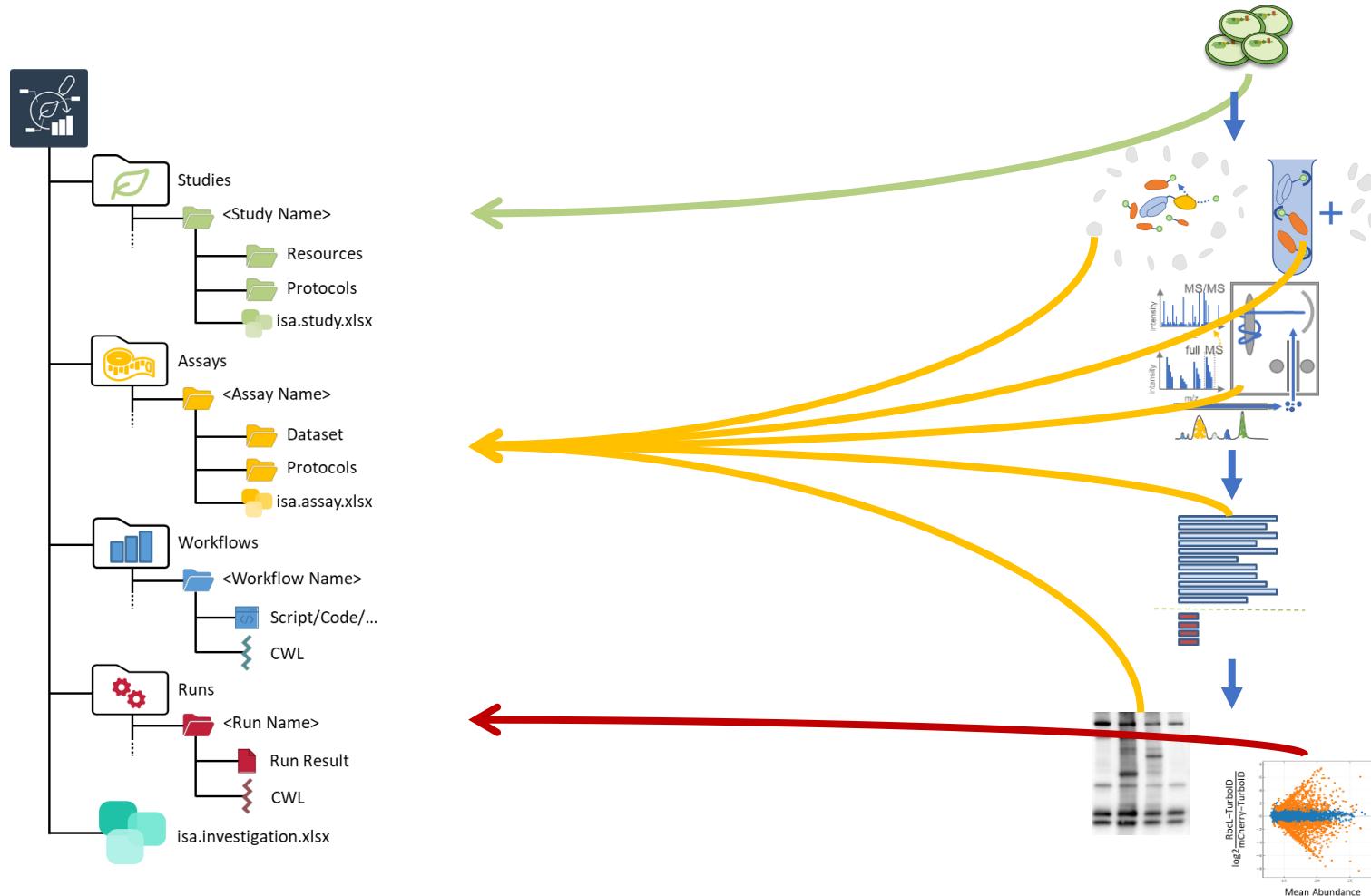


**Experimental
Data and
Meta Data**

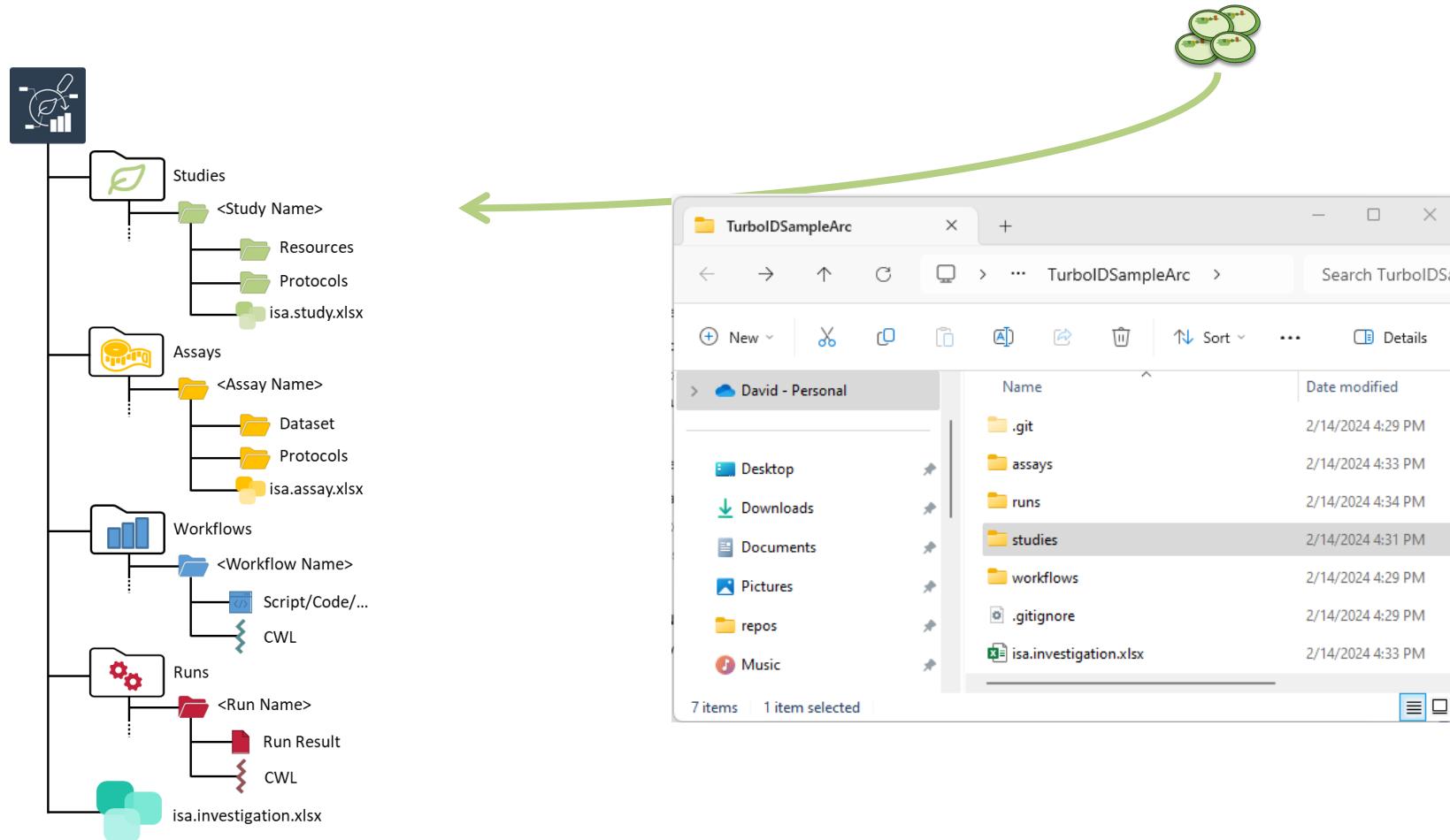
**Computational
Data and Meta
Data**



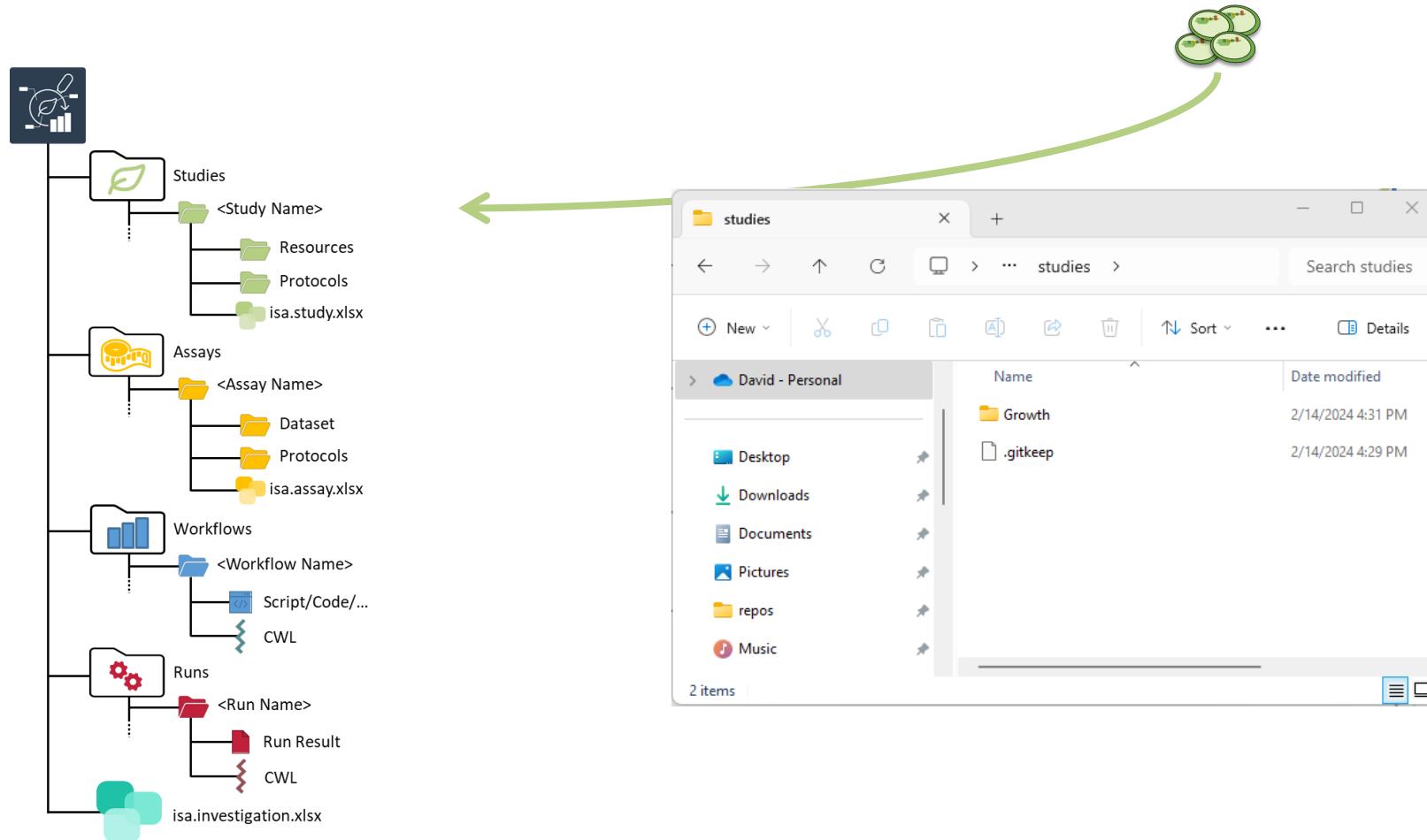
Important ARC Concepts: Structure and Data



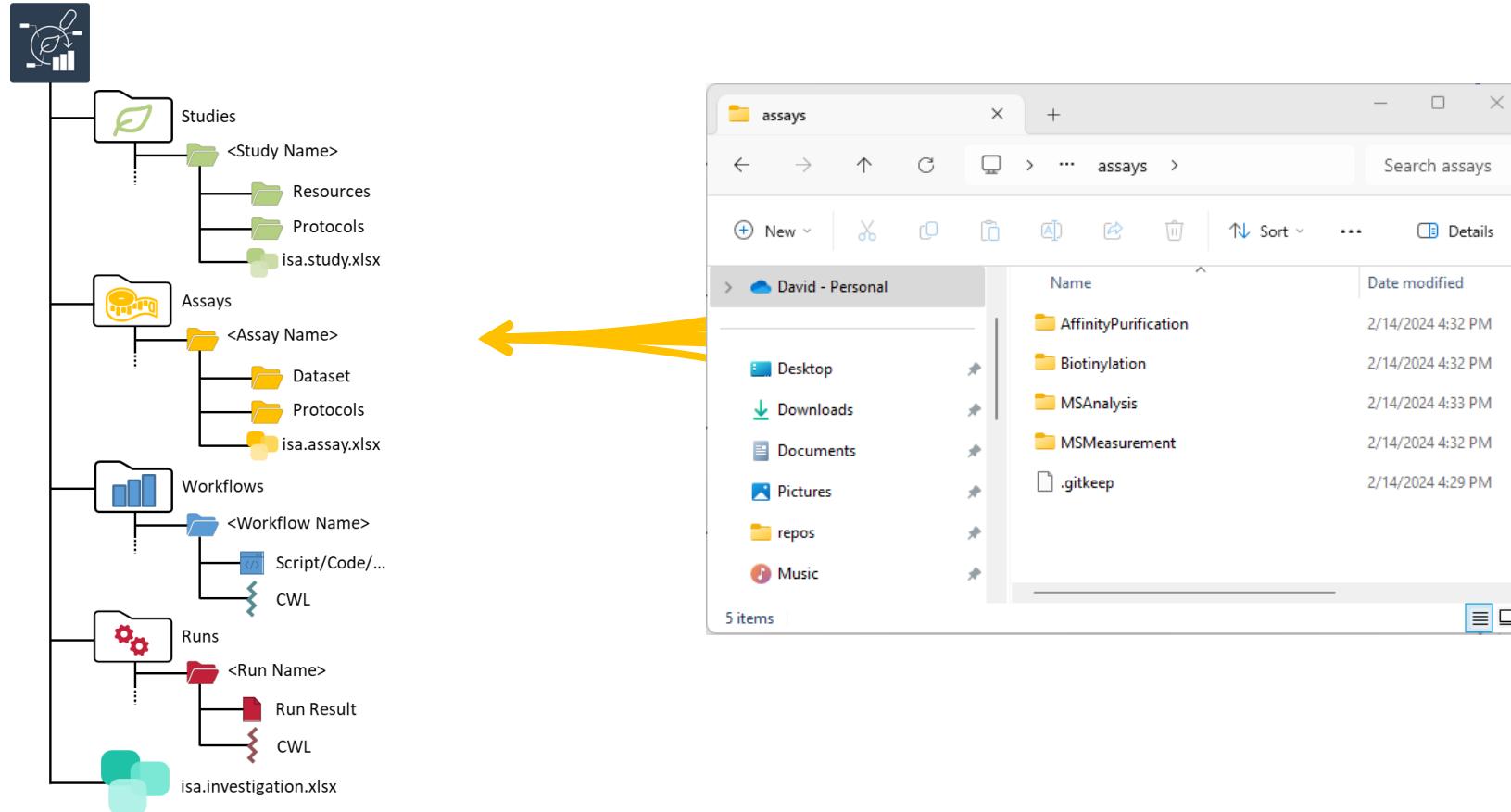
Important ARC Concepts: Structure and Data



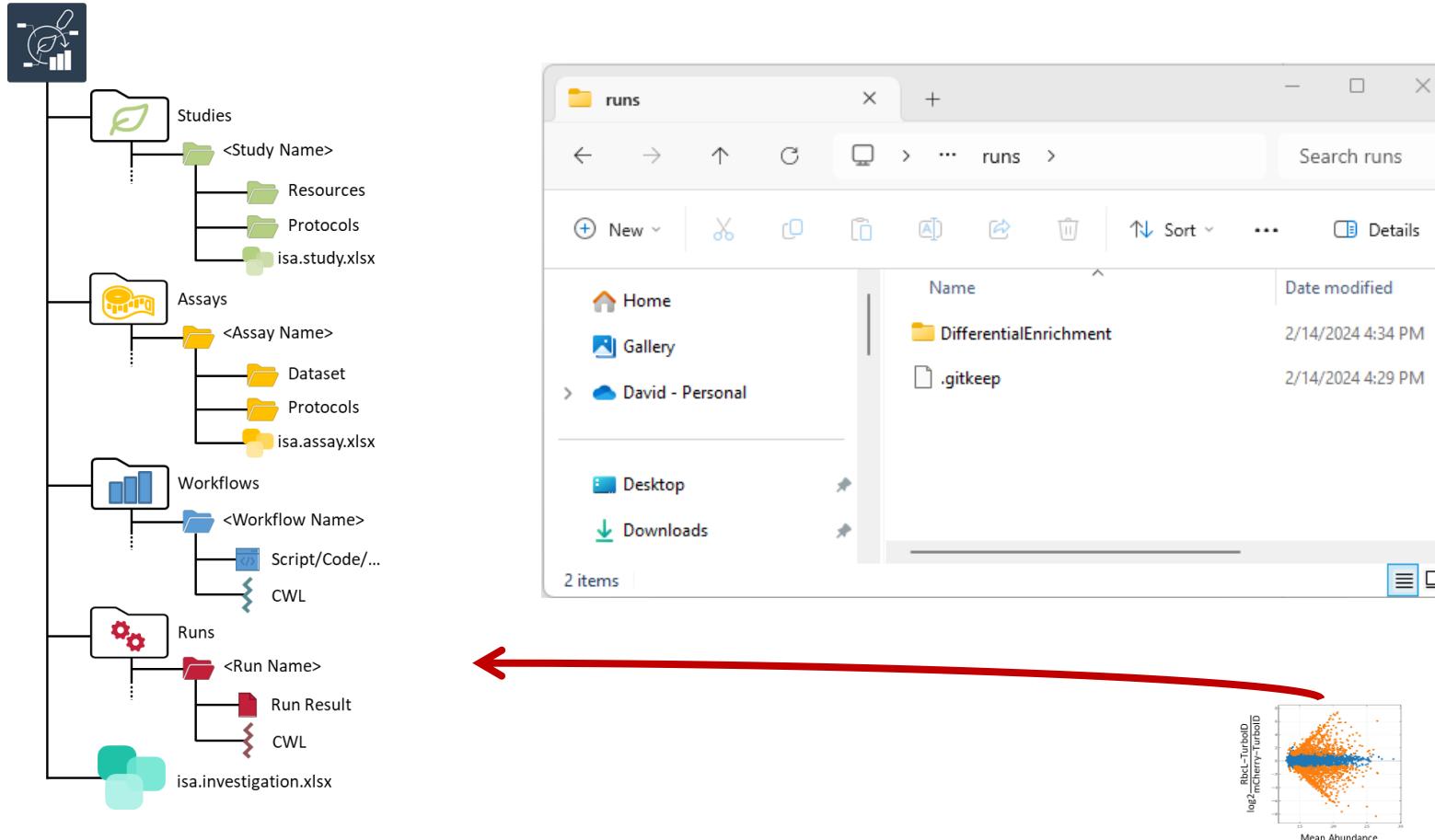
Important ARC Concepts: Structure and Data



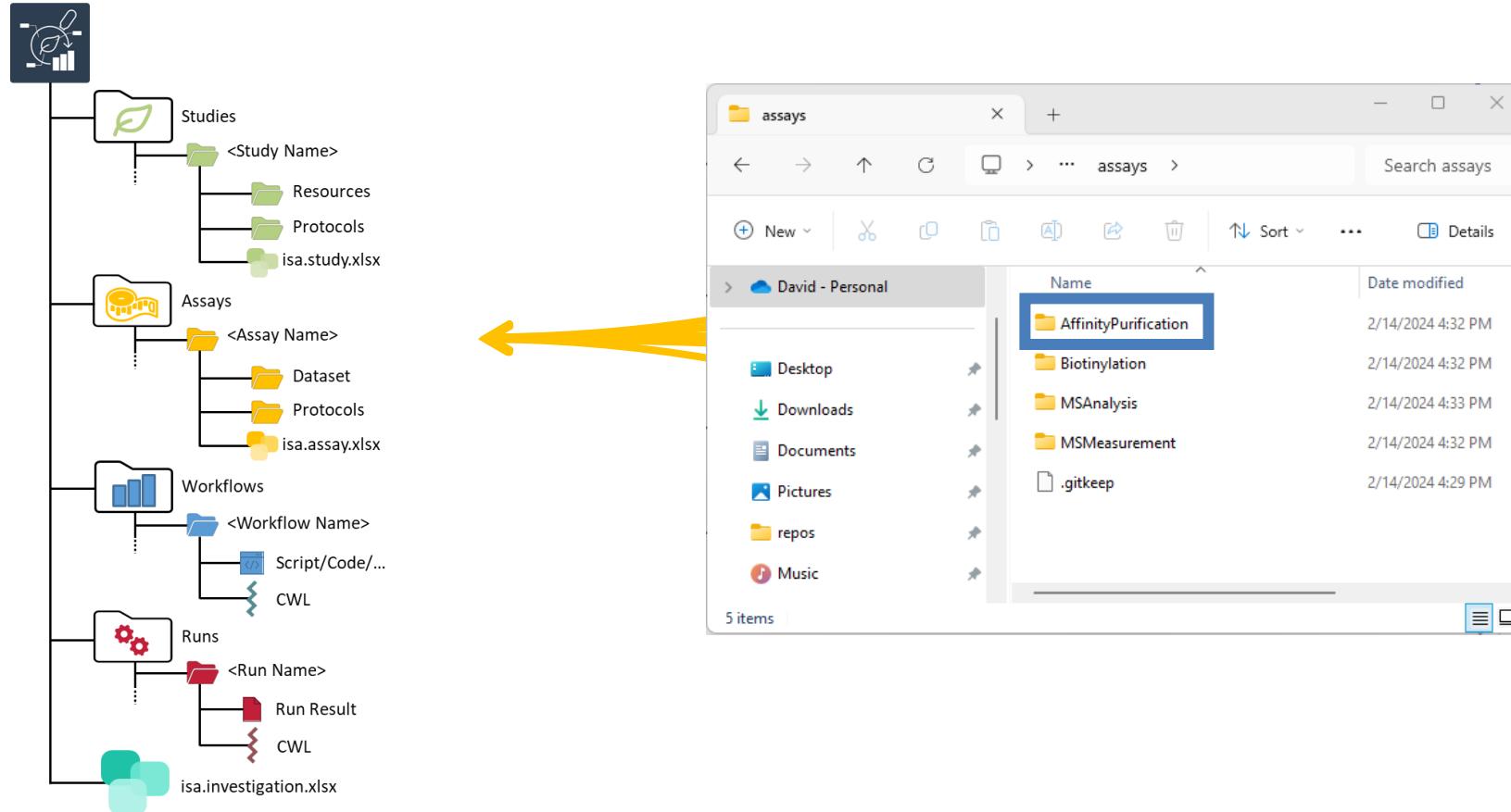
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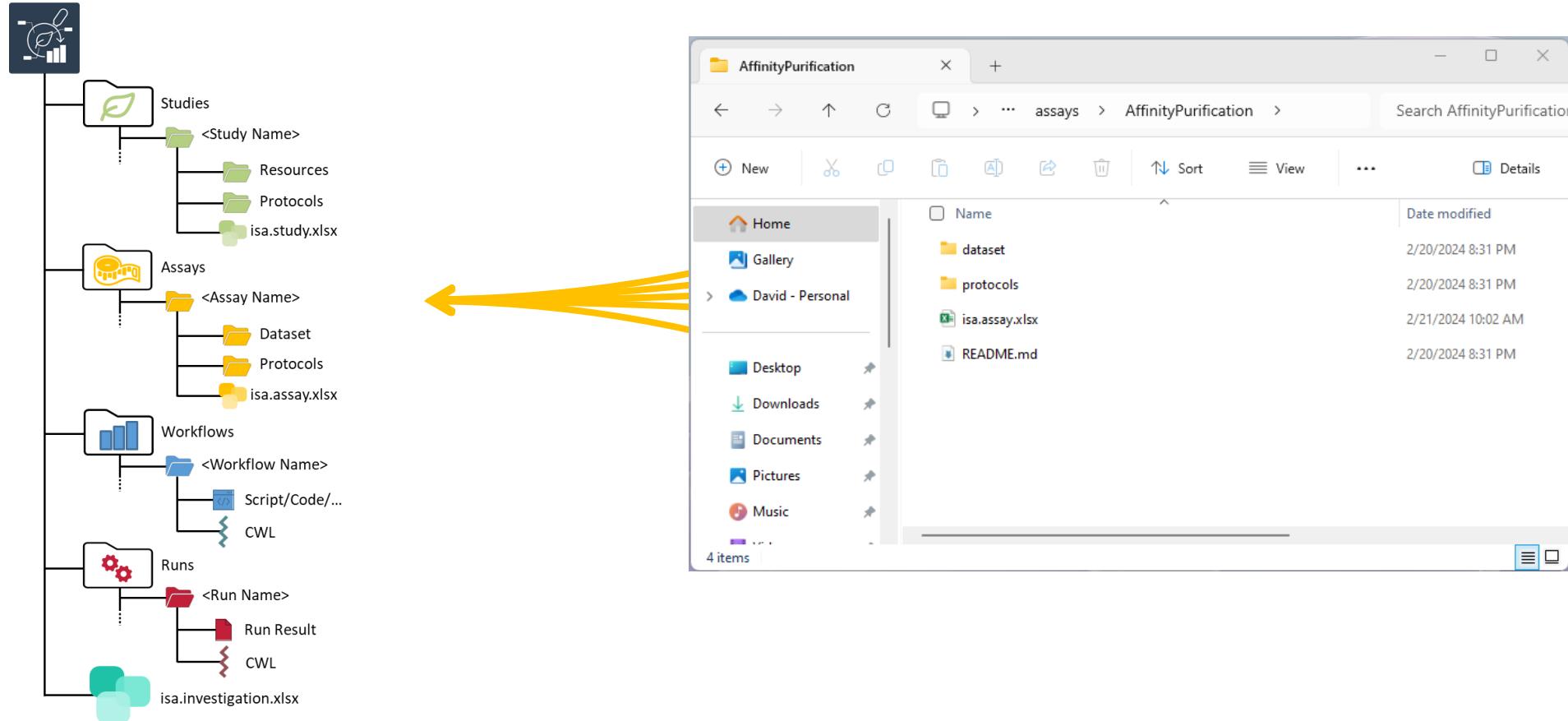
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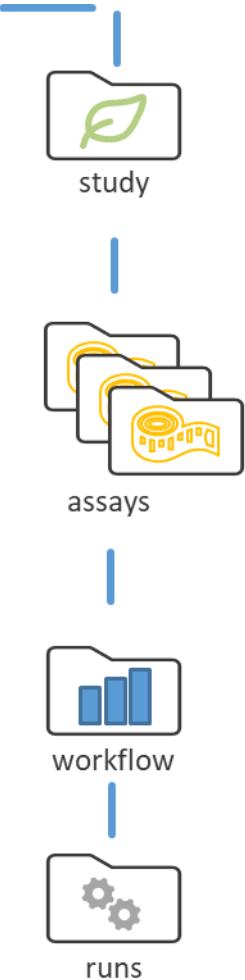
Important ARC Concepts: Structure and Data



Important ARC Concepts: Structure and Data



Agenda of part two

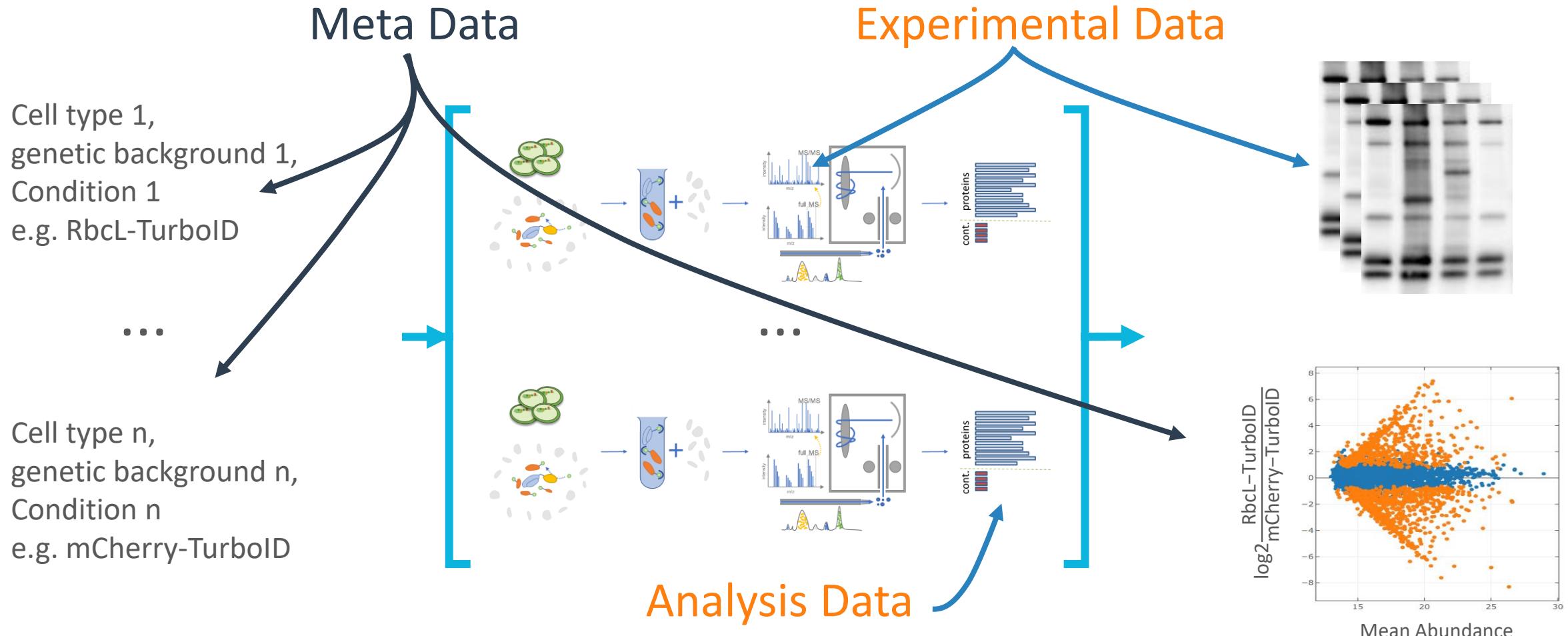


- I. Important ARC concepts by example:
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- II. Important ARC concepts by example:
Meta Data Annotation Principle
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PLANTDataHUB

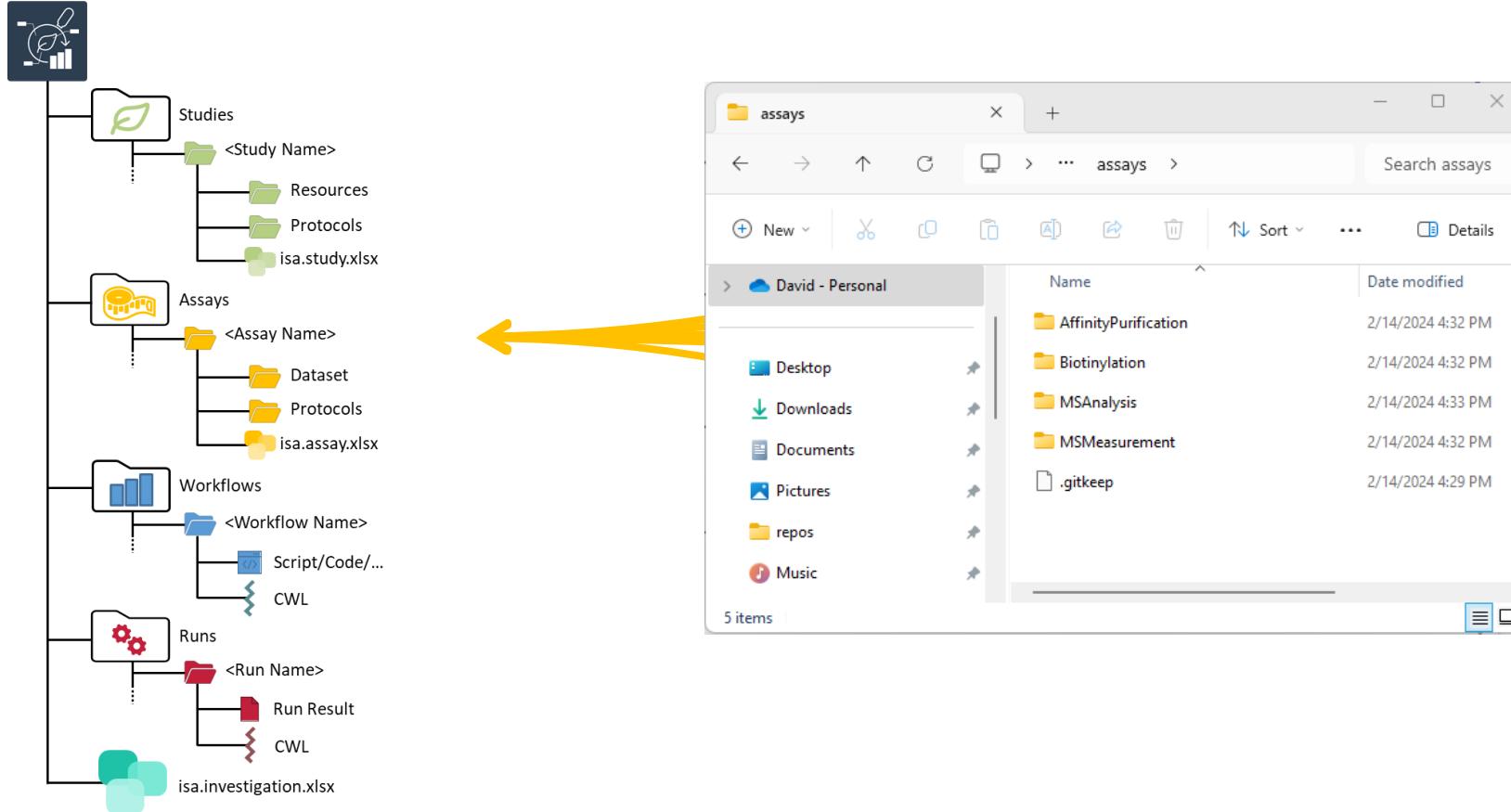
IV. Complete Walk-Through
using the ARCitect



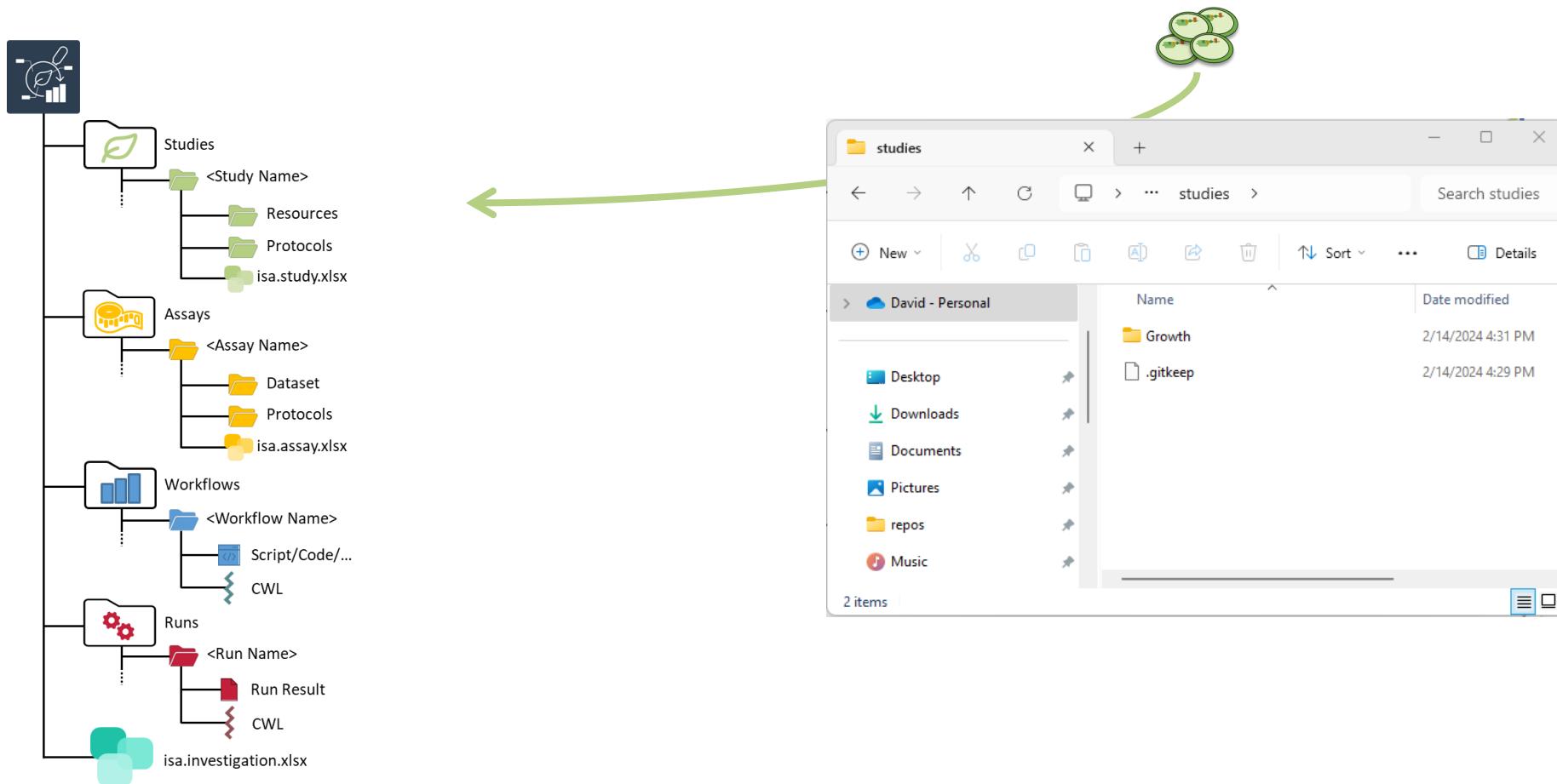
Motivation: An TurboID experiment



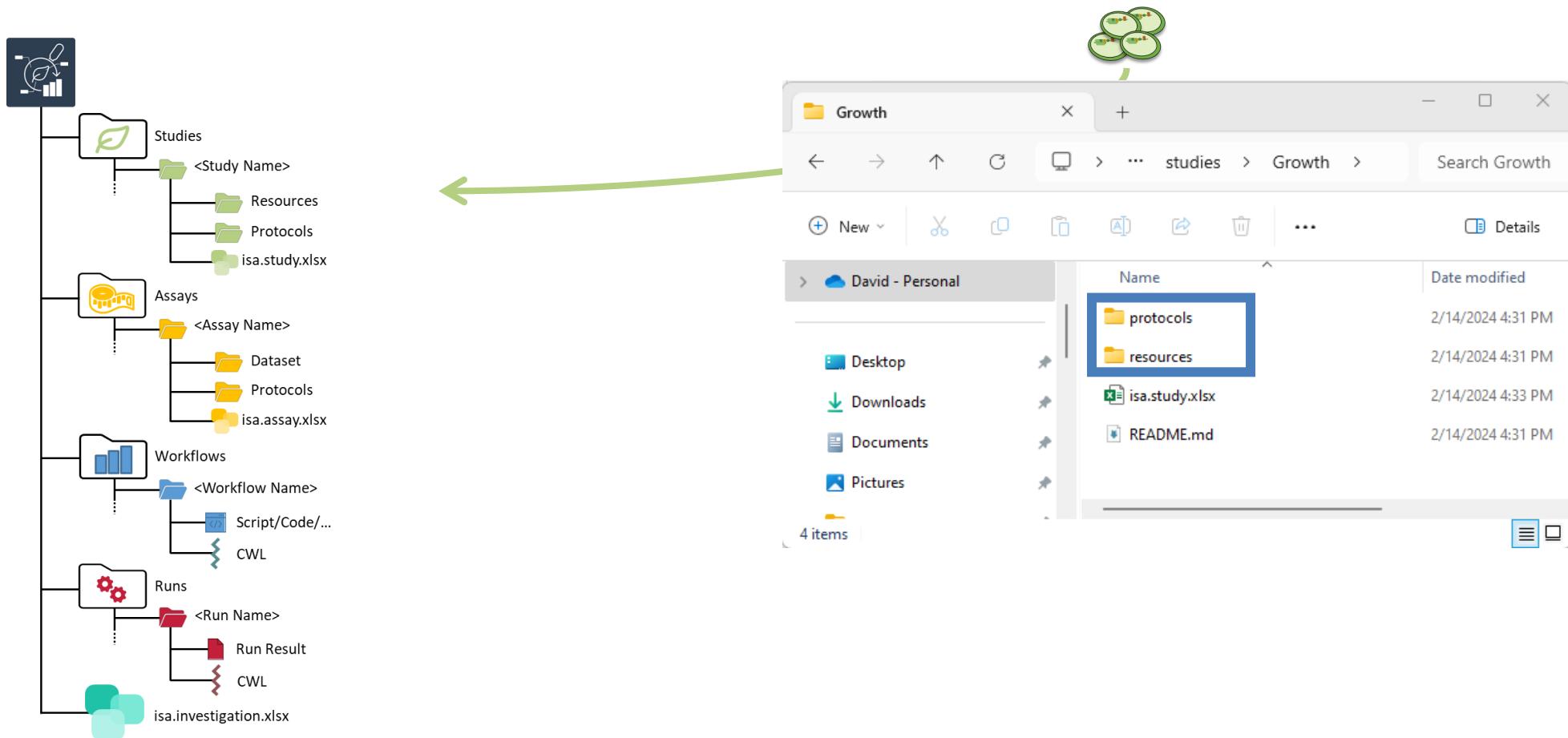
Important ARC Concepts: Meta Data



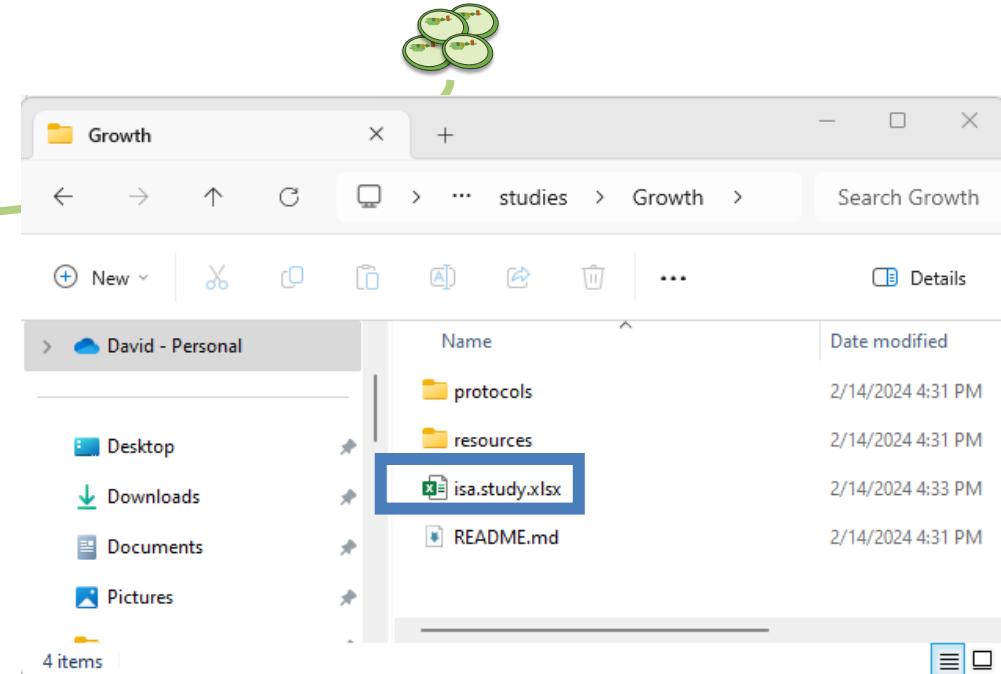
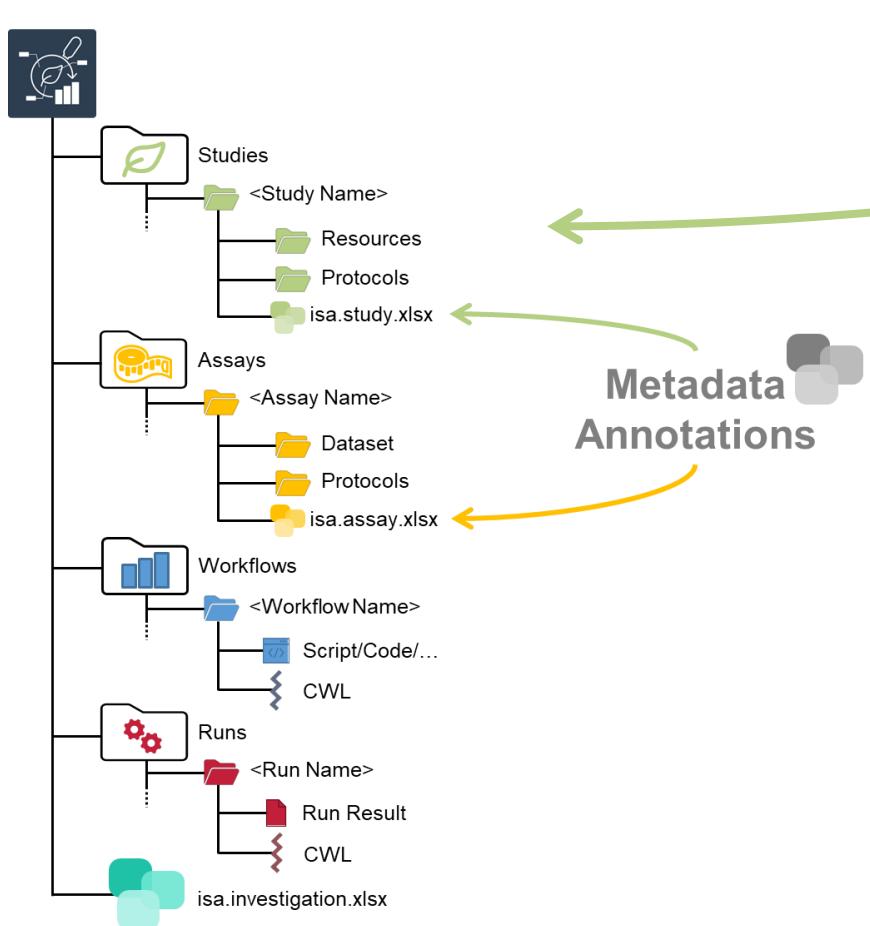
Important ARC Concepts: Meta Data



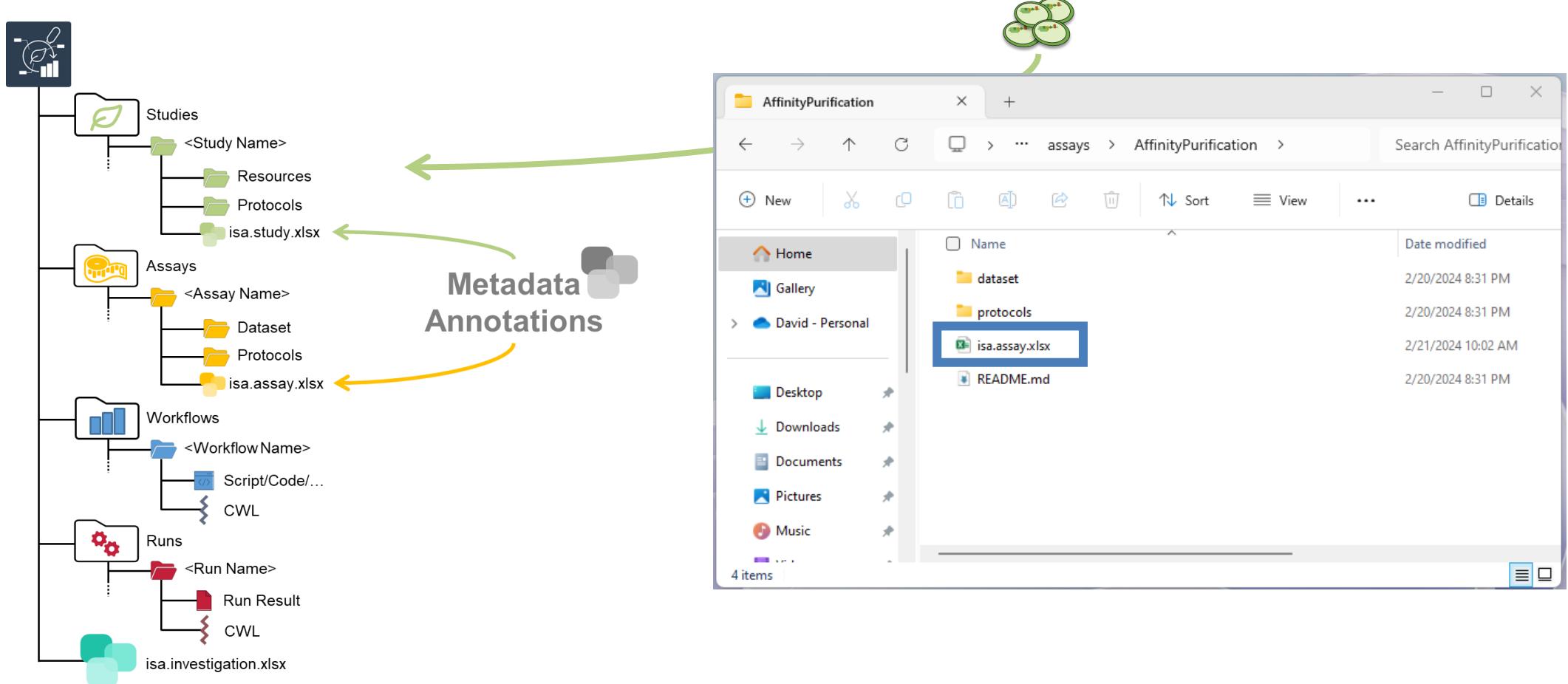
Important ARC Concepts: Meta Data



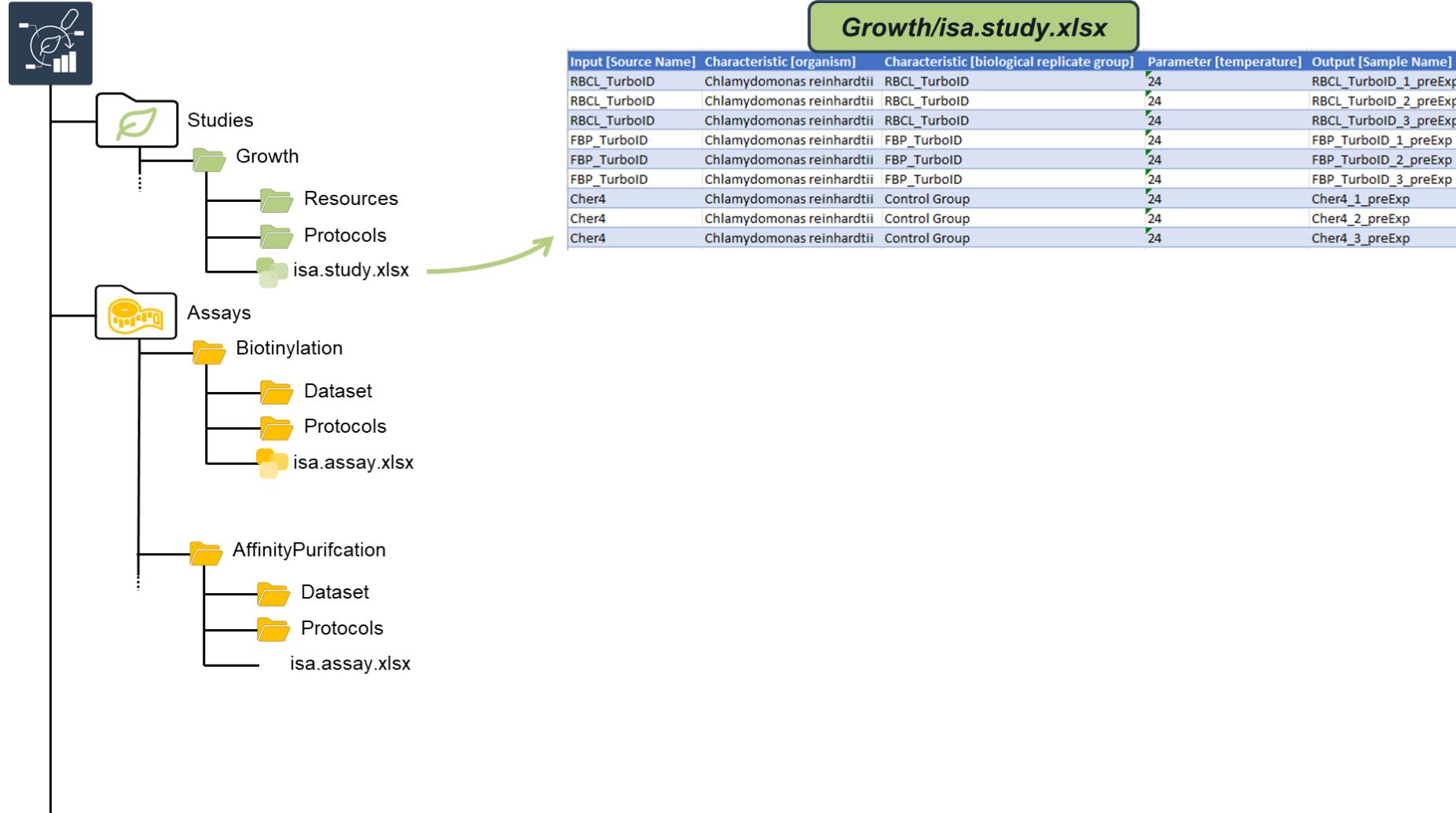
Important ARC Concepts: Meta Data



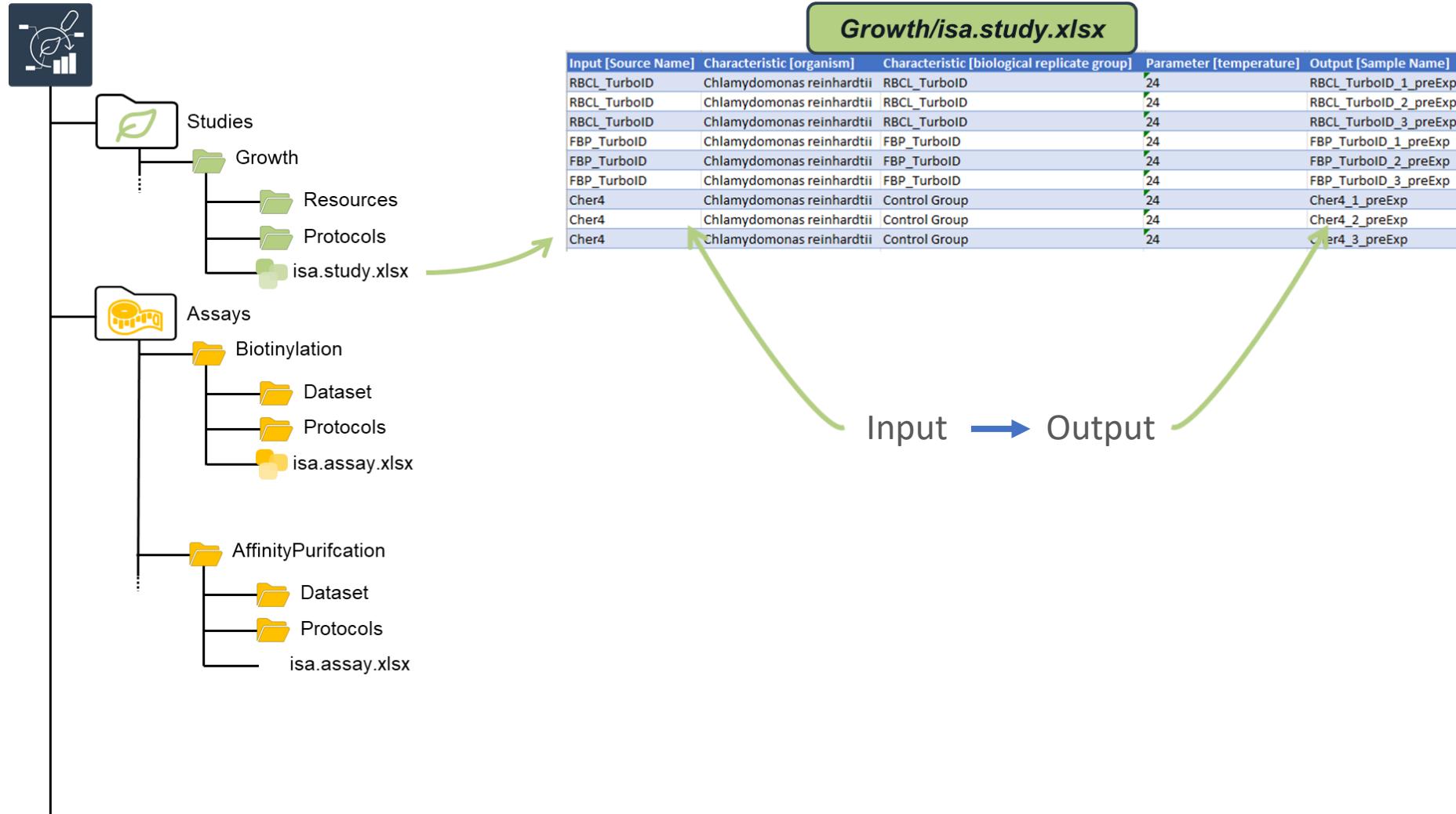
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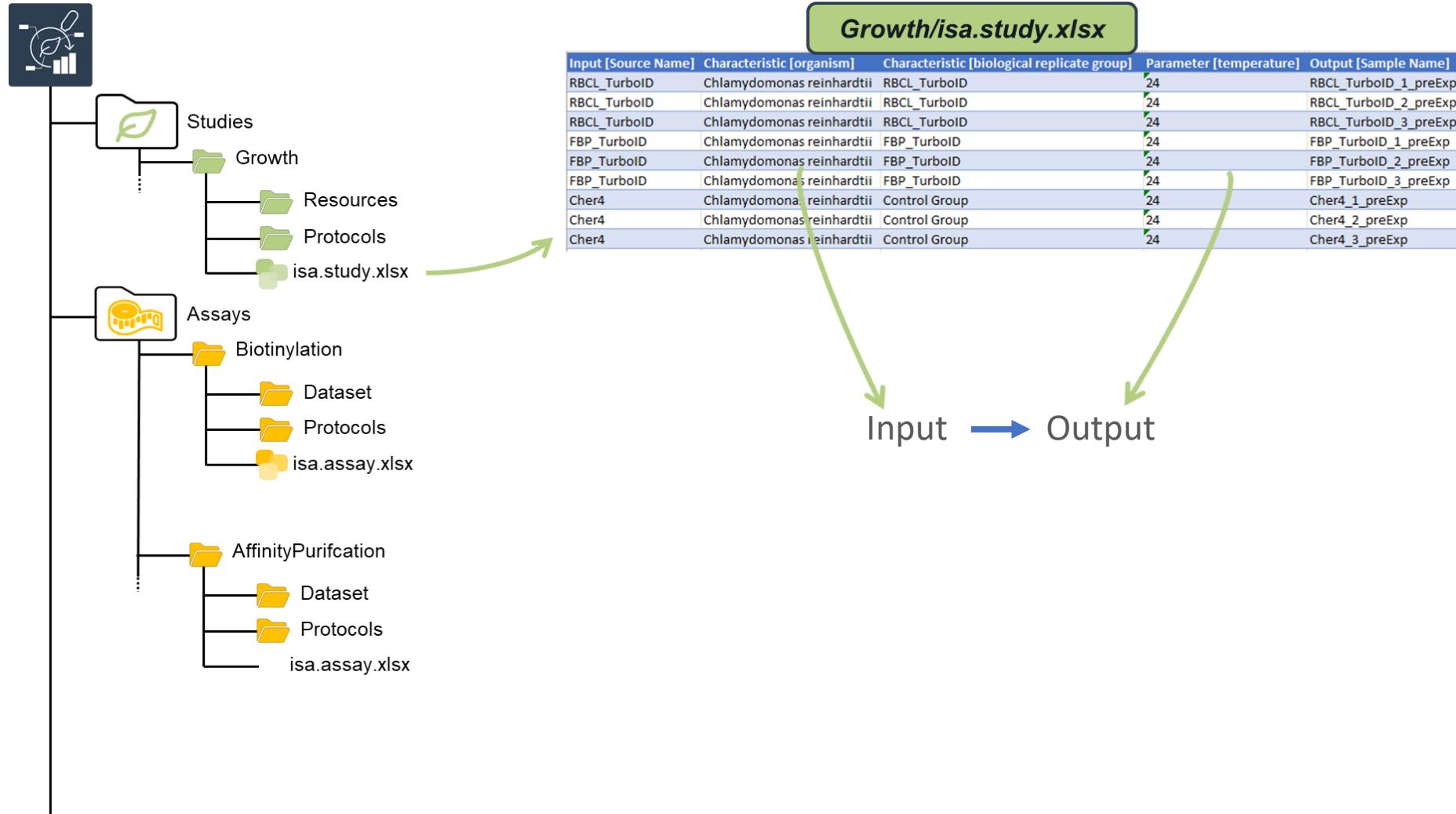
Important ARC Concepts: Meta Data



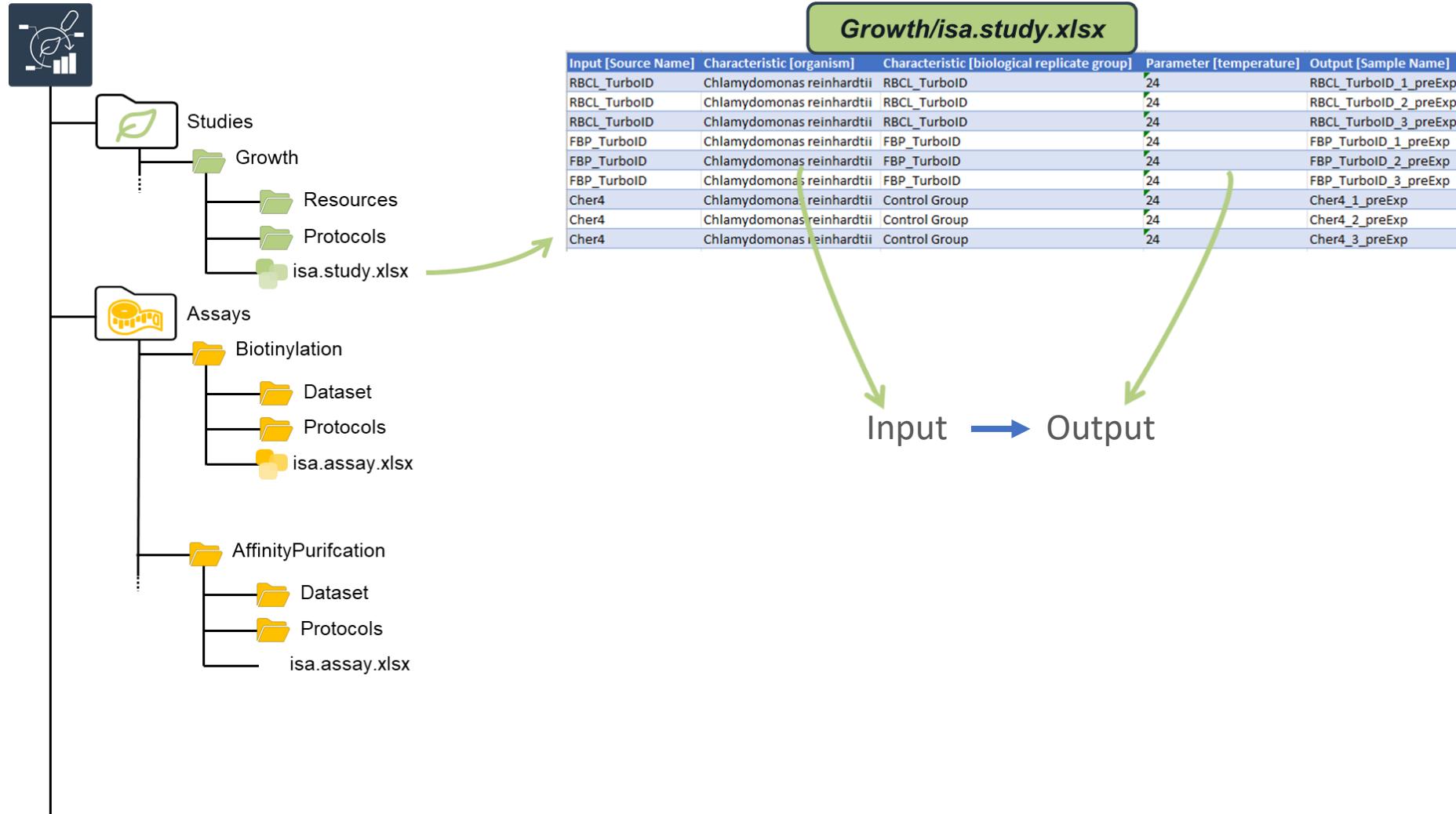
Important ARC Concepts: Meta Data



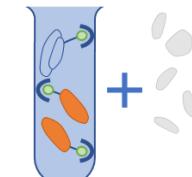
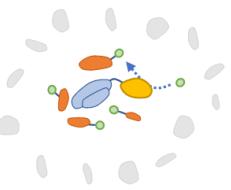
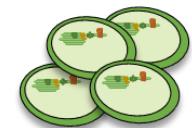
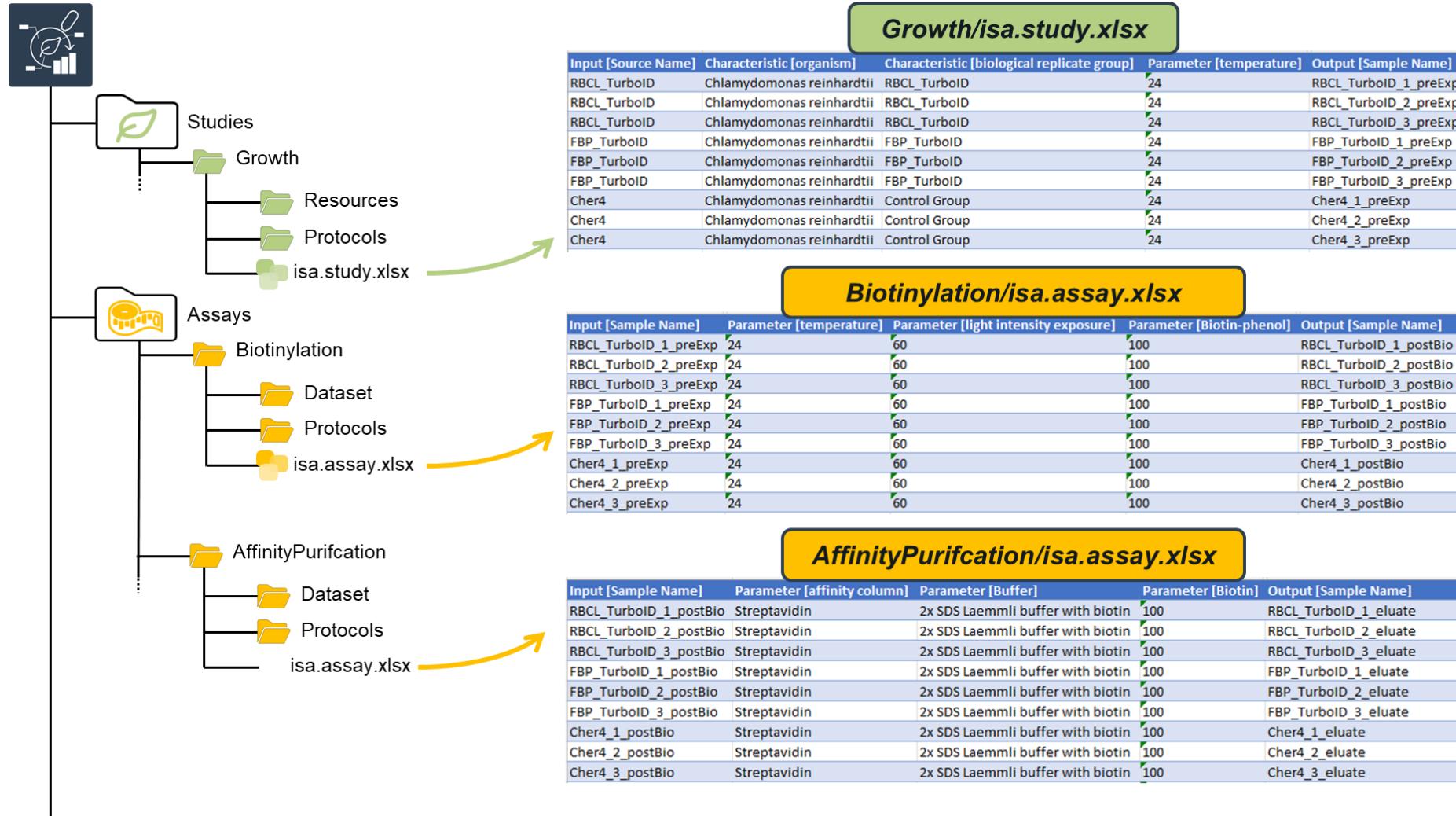
Important ARC Concepts: Meta Data



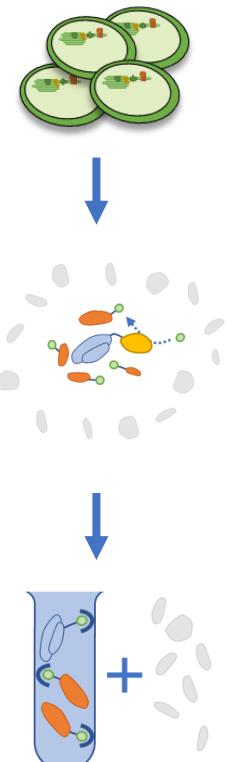
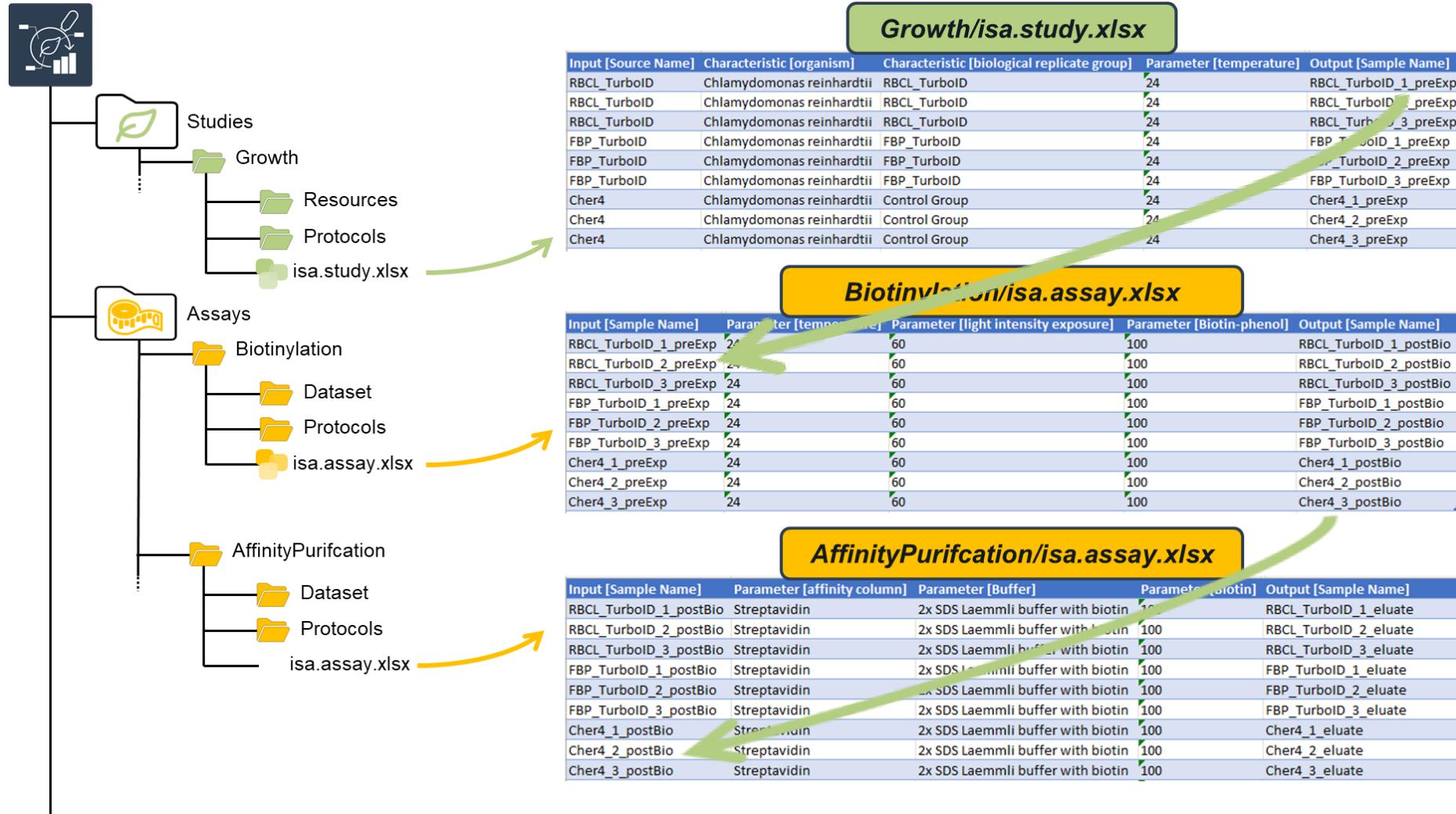
Important ARC Concepts: Meta Data



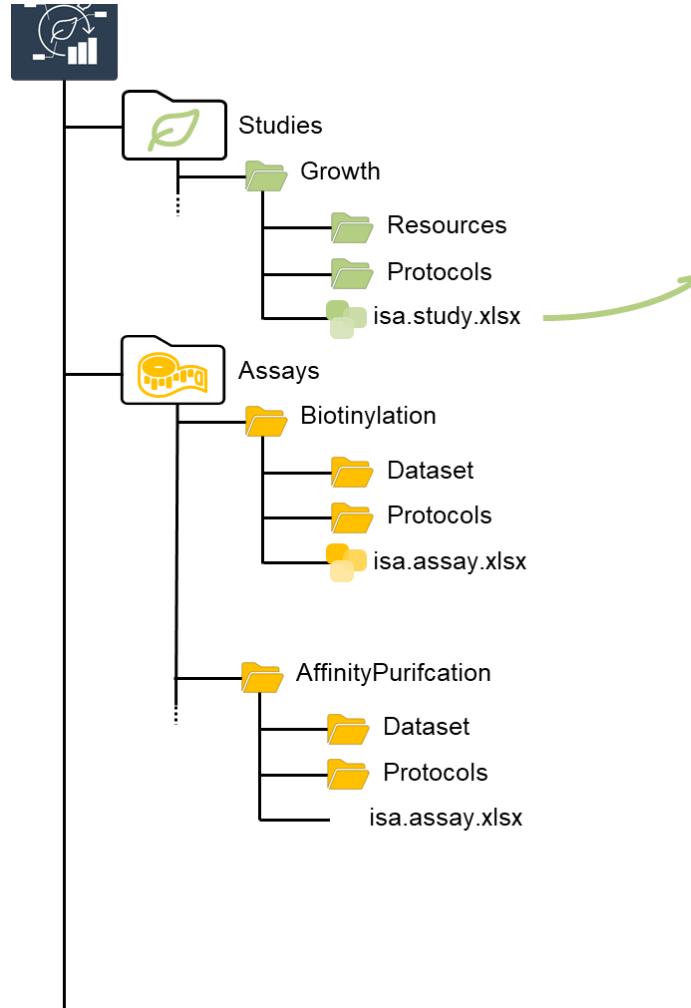
Important ARC Concepts: Meta Data



Important ARC Concepts: Meta Data



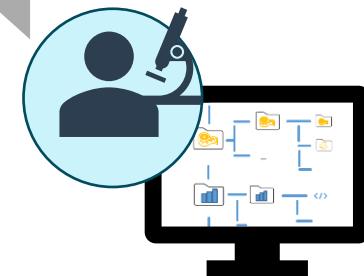
Important ARC Concepts: Meta Data



Input [Source Name]	Character
RBCL_TurboID	Chlamy
RBCL_TurboID	Chlamy
RBCL_TurboID	Chlamy
FBP_TurboID	Chlamy
FBP_TurboID	Chlamy
FBP_TurboID	Chlamy
Cher4	Chlamy
Cher4	Chlamy
Cher4	Chlamy

Q: Ok, great! But how is this FAIR? I do not know how you defined „temperature“, or what the unit of the value 24 is?

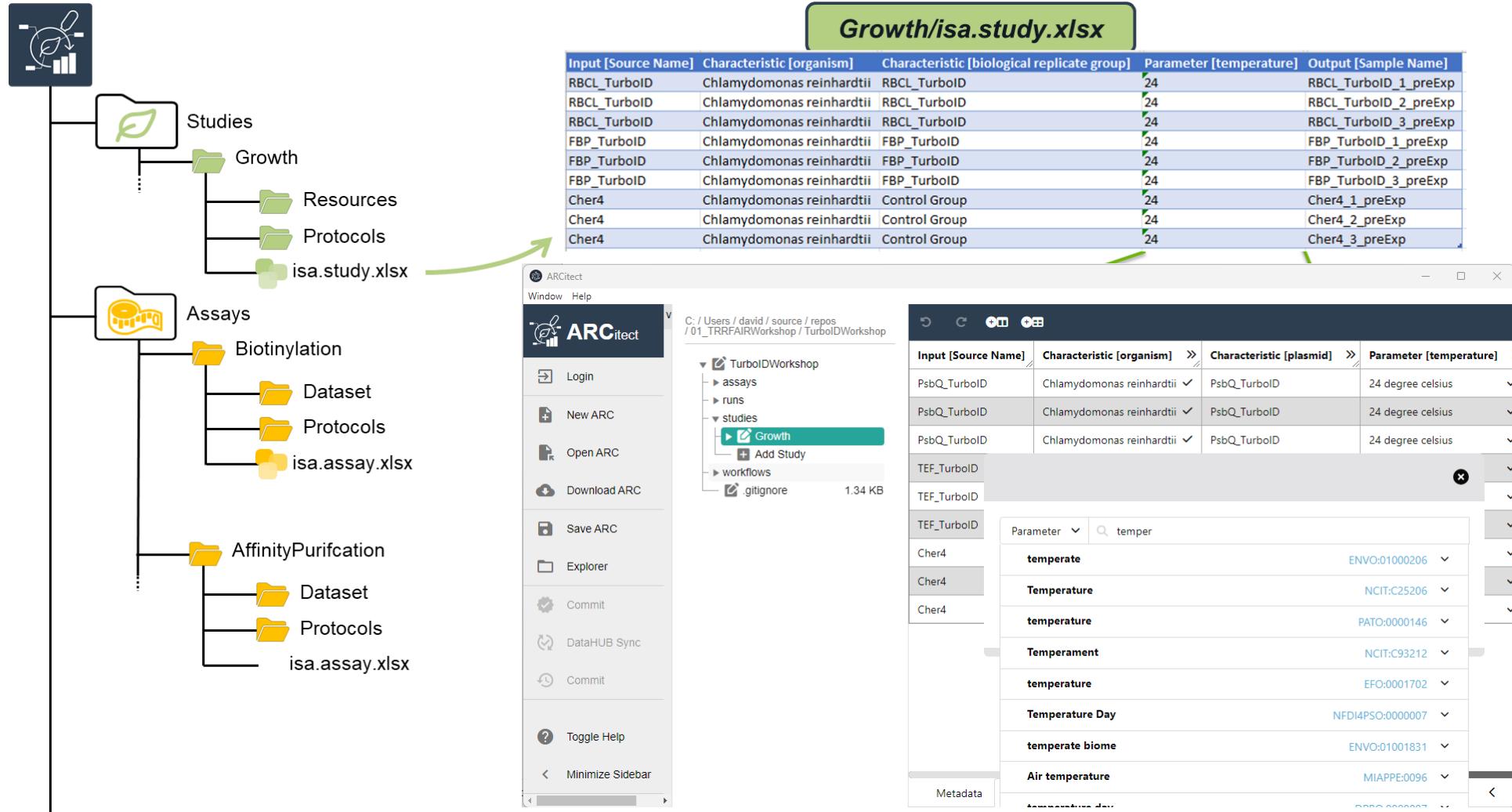
perature	Output [Sample Name]
RBCL_TurboID_1	preExp
RBCL_TurboID_2	preExp
RBCL_TurboID_3	preExp
FBP_TurboID_1	preExp
FBP_TurboID_2	preExp
FBP_TurboID_3	preExp
Cher4_1	preExp
Cher4_2	preExp
Cher4_3	preExp



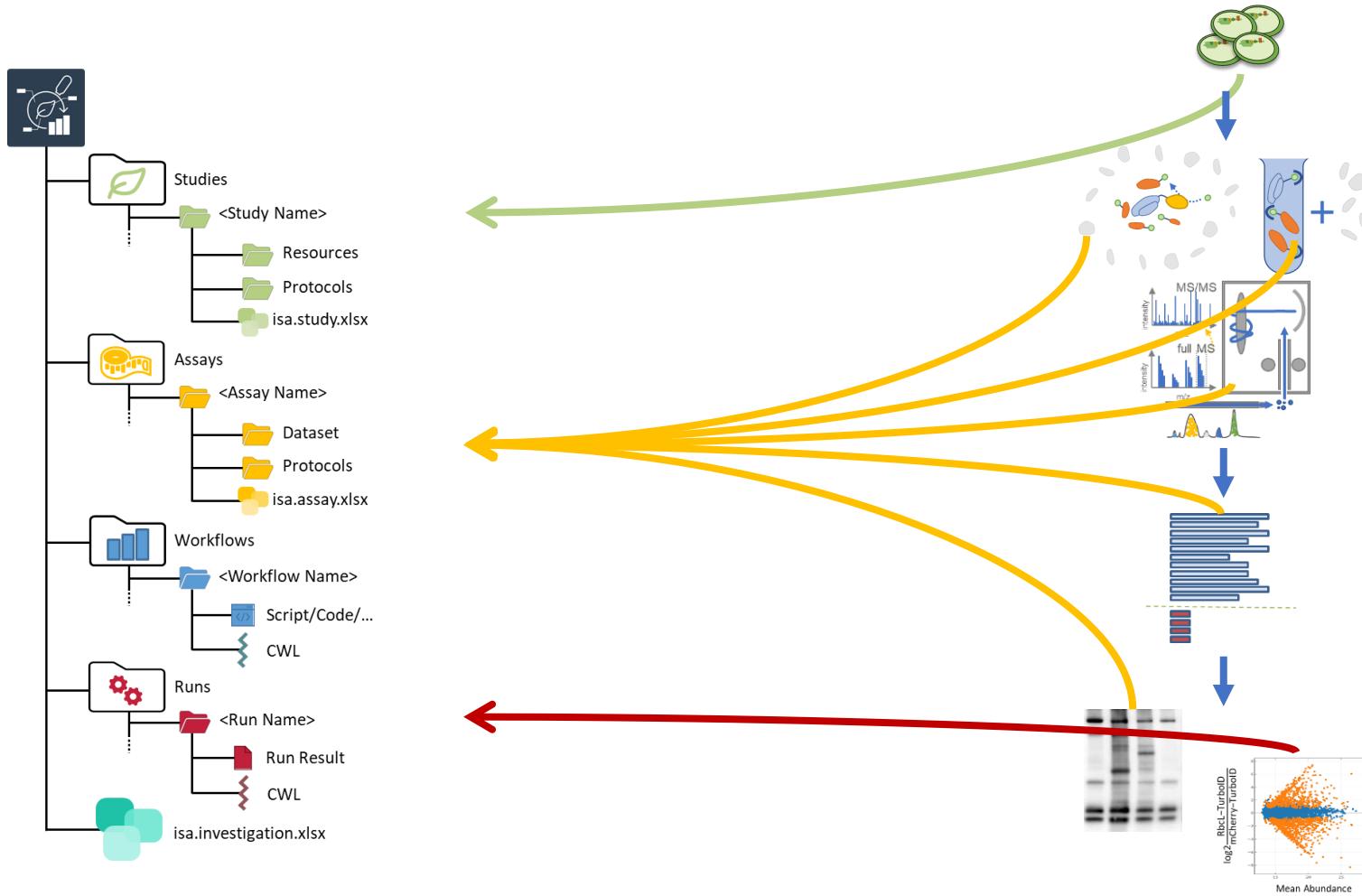
Important ARC Concepts: Meta Data



Important ARC Concepts: Meta Data



Important ARC Concepts: Meta Data



Agenda of part two



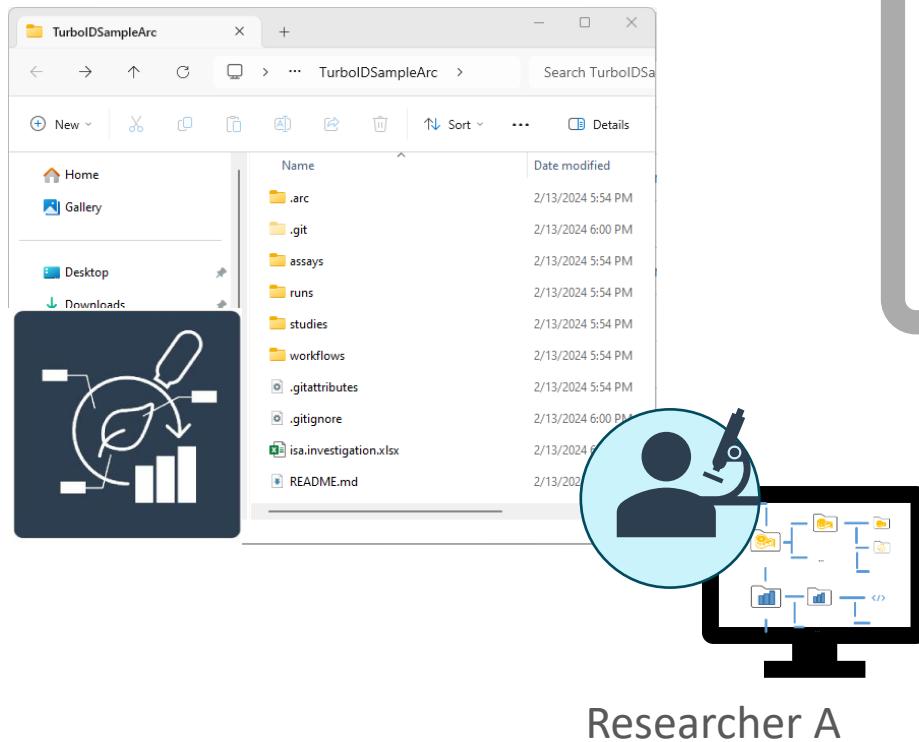
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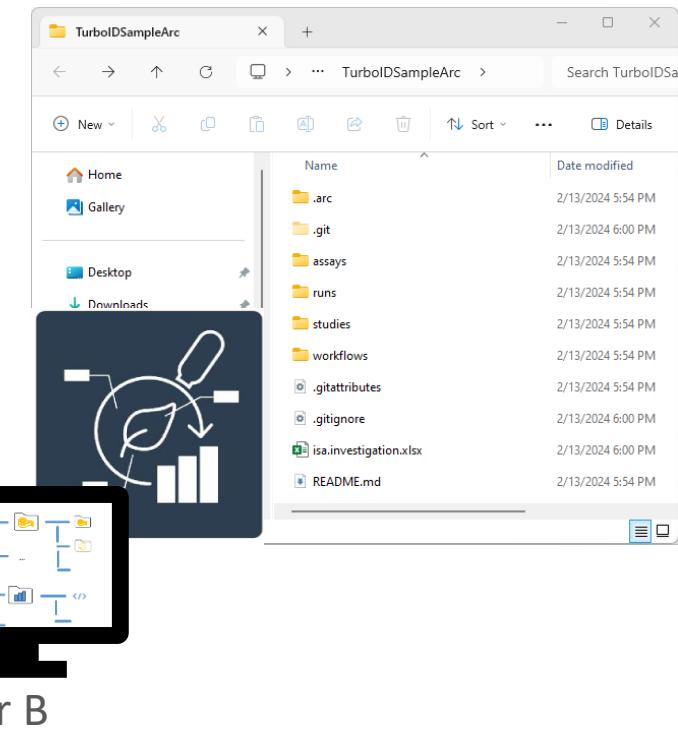


Now: ARCs as a single RDM entry point

Researcher As data management solution:
Annotated Research Context (ARC)



Researcher Bs data management solution:
Annotated Research Context (ARC)

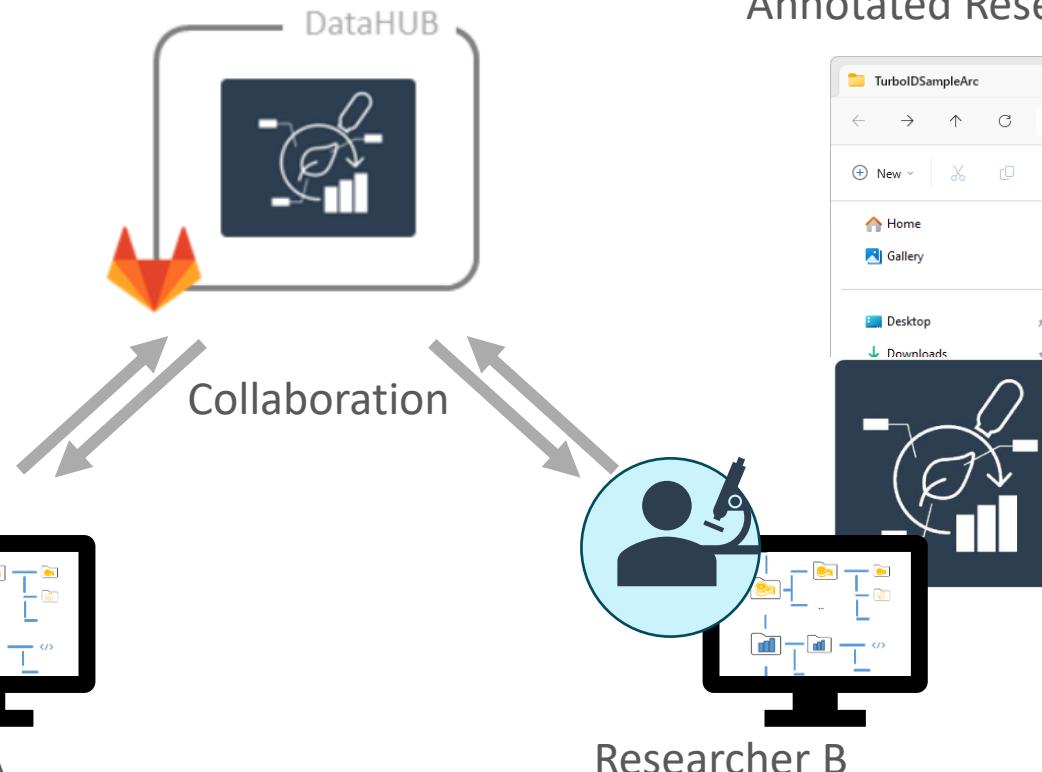
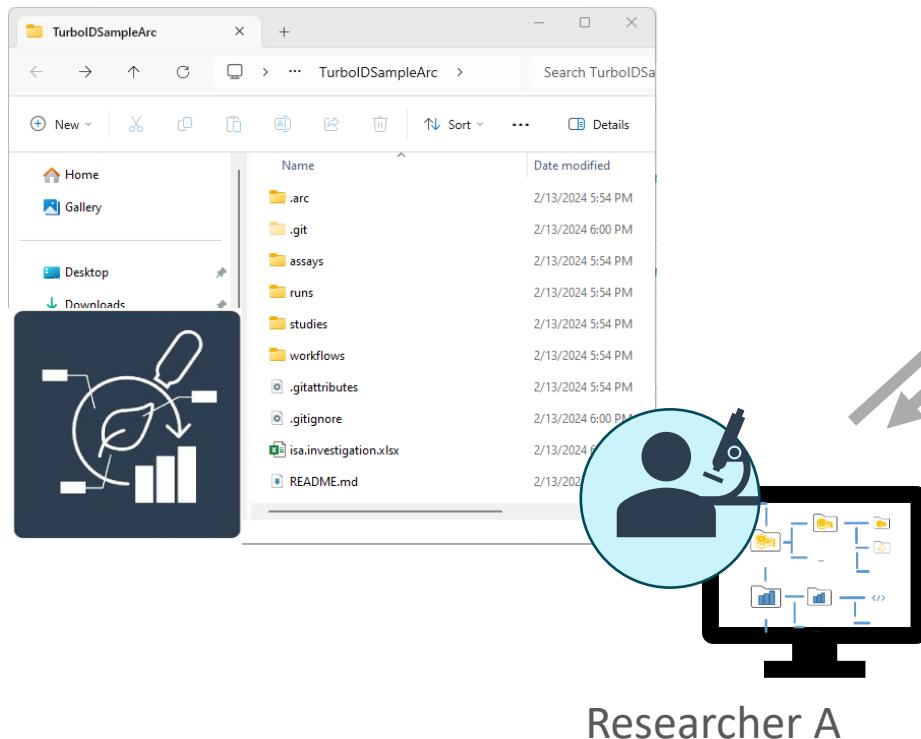


How do we
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Any Updates?

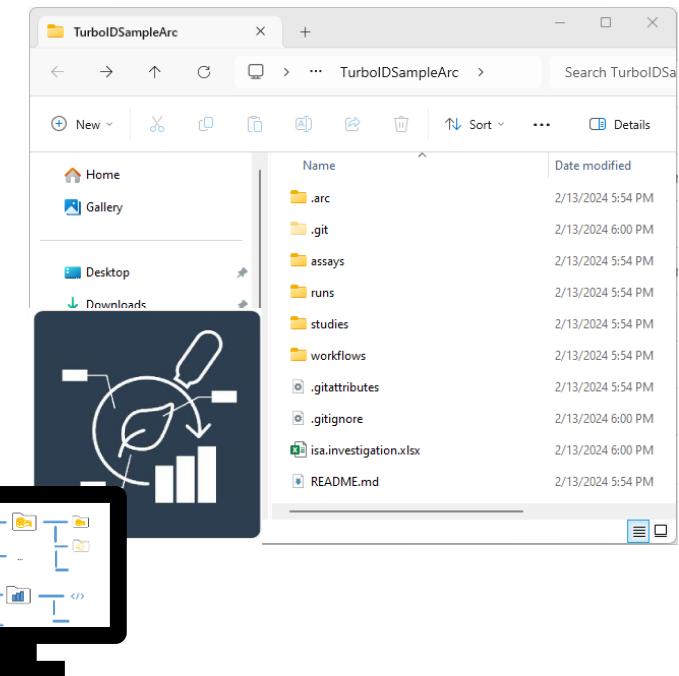
Collaboration

Now: Using the PLANTDataHUB to collaborate

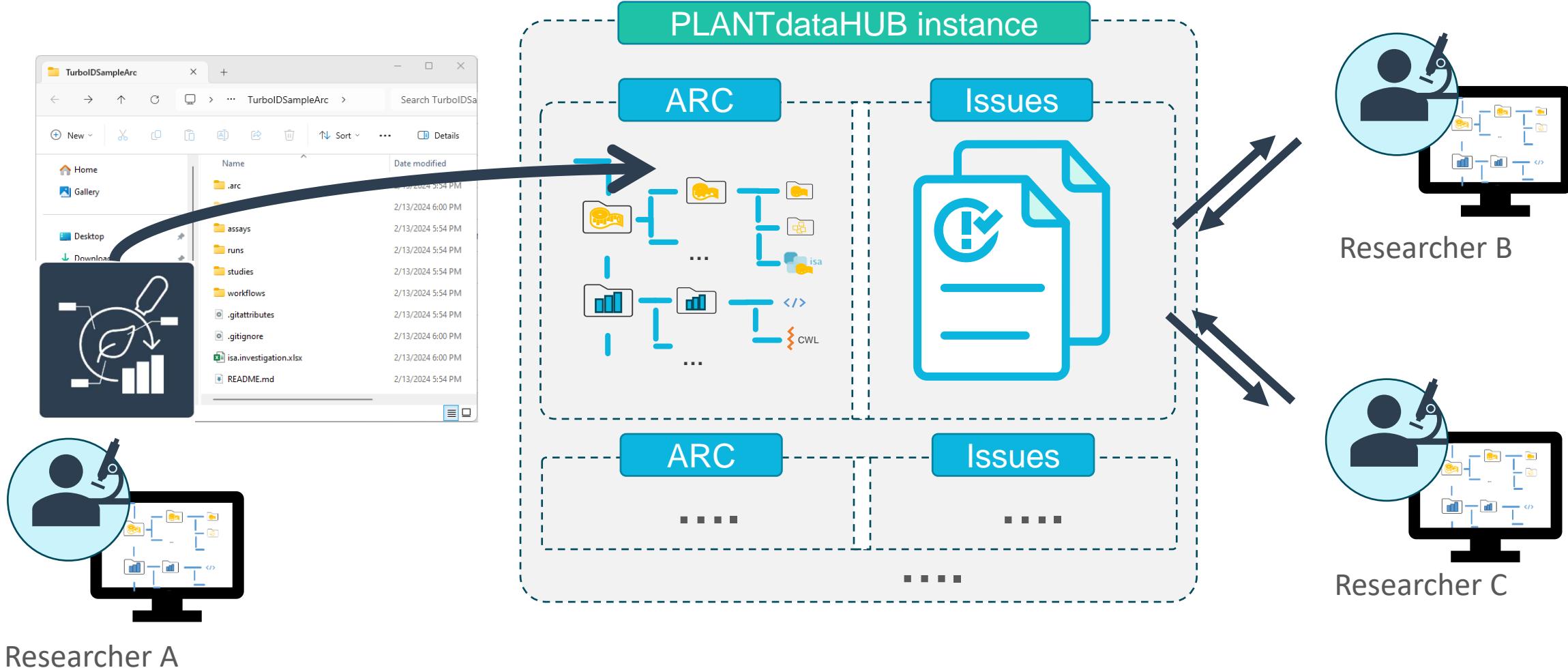
Researcher As data management solution:
Annotated Research Context (ARC)



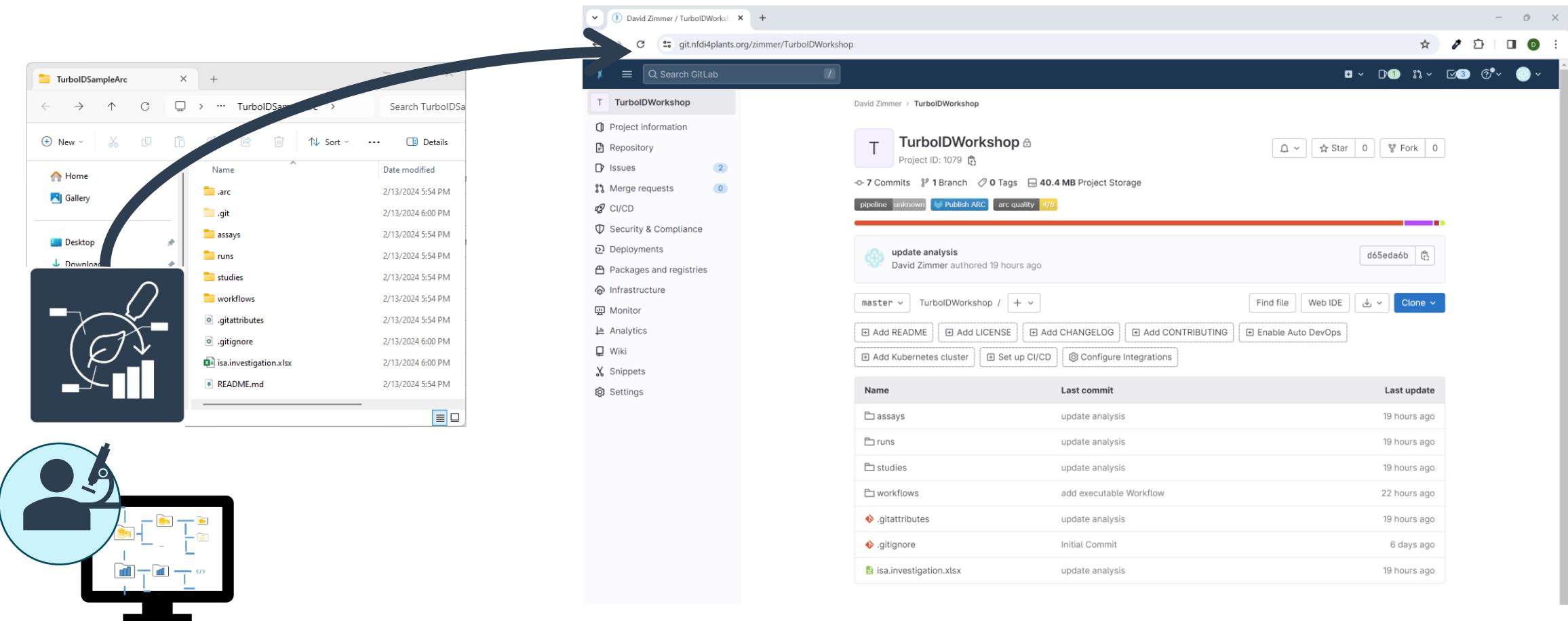
Researcher Bs data management solution:
Annotated Research Context (ARC)



Now: Using the PLANTDataHUB to collaborate



Now: Using the PLANTDataHUB to collaborate



Researcher A

Now: Using the PLANTDataHUB to collaborate

The diagram illustrates the collaboration process between Researcher A and the PLANTDataHUB.

Researcher A's Environment: On the left, a screenshot of the TurboIDSampleArc software interface is shown. It displays a file tree with various project files like .arc, .git, assays, runs, studies, workflows, .gitattributes, .gitignore, isa.investigation.xlsx, and README.md. Below the file tree is a large icon depicting a plant sample being analyzed by a mass spectrometer, with bar charts representing the resulting data.

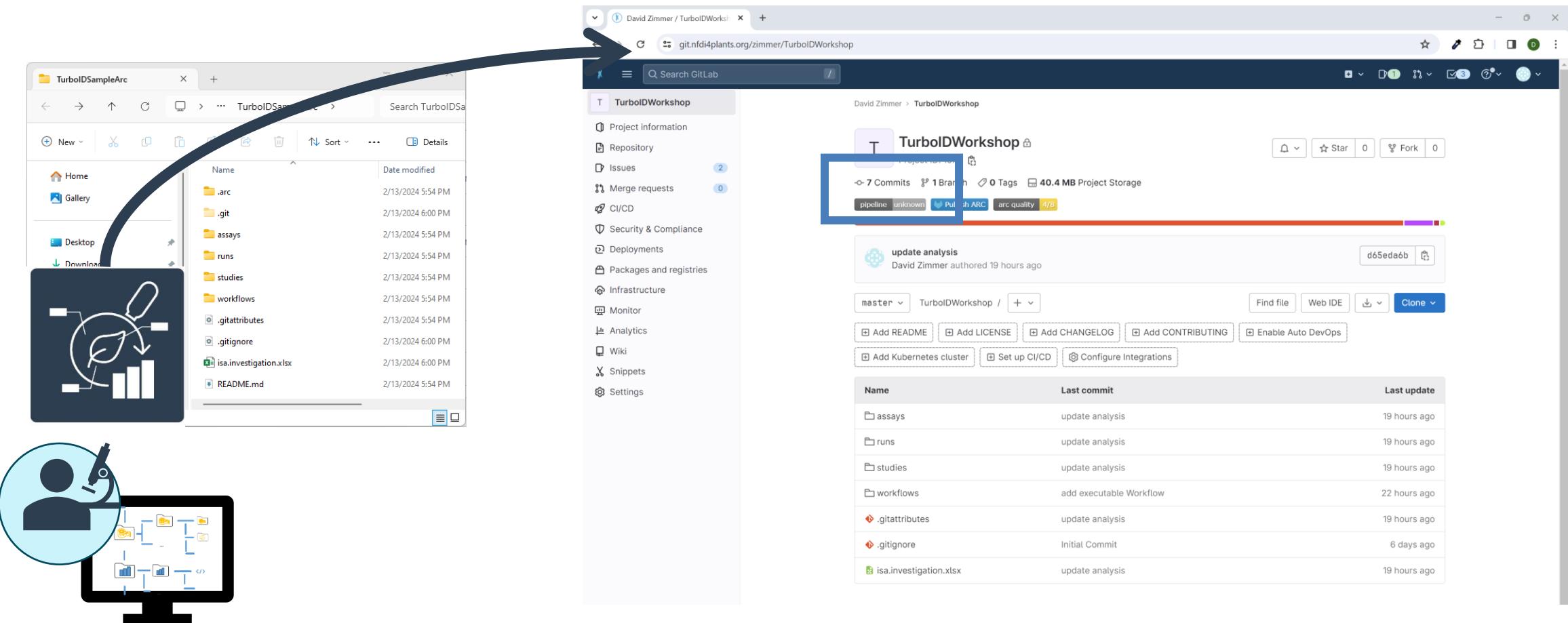
Collaboration Platform: On the right, a screenshot of the GitLab interface for the TurboIDWorkshop project is shown. The URL in the address bar is git.nfdi4plants.org/zimmer/TurboIDWorkshop/-/tree/master/assays. The sidebar shows project navigation options: Project information, Repository, Issues (2), Merge requests (0), CI/CD, Security & Compliance, Deployments, Packages and registries, Infrastructure, Monitor, Analytics, Wiki, Snippets, and Settings. The main content area shows a recent update from David Zimmer: "update analysis" authored 20 hours ago. Below this is a list of files in the master branch, each with its last commit details:

Name	Last commit	Last update
..		
AffinityPurification	update analysis	20 hours ago
Biotinylation	update analysis	20 hours ago
MSAnalysis	update analysis	20 hours ago
MSMeasurement	update analysis	20 hours ago
Western	update analysis	20 hours ago
.gitkeep	Initial Commit	6 days ago

A large blue arrow points from the TurboIDSampleArc interface towards the GitLab interface, indicating the flow of data or collaboration between the two environments.

Researcher A

Now: Using the PLANTDataHUB to collaborate



Researcher A

Now: Using the PLANTDataHUB to collaborate

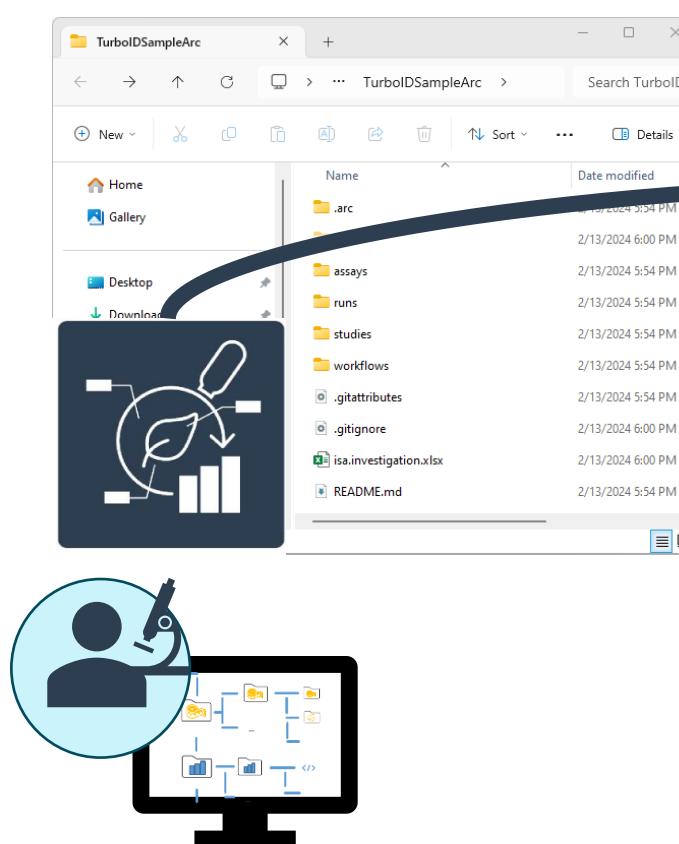
The screenshot illustrates the integration of the PLANTDataHUB with a GitLab repository. On the left, a file browser window titled "TurboIDSampleArc" shows a directory structure with files like ".arc", ".git", "assays", "runs", "studies", "workflows", ".gitattributes", ".gitignore", "isa.investigation.xlsx", and "README.md". A large blue arrow points from this browser to the right-hand GitLab interface. The GitLab interface displays the "Commits" page for the "TurboIDWorkshop" project. The sidebar includes links for "Project information", "Repository", "Commits" (which is selected), "Branches", "Tags", "Contributors", "Graph", "Compare", "Issues", "Merge requests", "CI/CD", "Security & Compliance", "Deployments", "Packages and registries", "Infrastructure", "Monitor", "Analytics", "Wiki", "Snippets", and "Settings". The main content area shows a list of commits:

- 21 Feb, 2024 4 commits
 - update analysis
David Zimmer authored 20 hours ago
d65eda6b
 - add executable Workflow
David Zimmer authored 23 hours ago
15497a2a
 - add meta data, add workflow
David Zimmer authored 1 day ago
db2a4e0c
 - add legacy workflow
David Zimmer authored 1 day ago
2d16124d
- 20 Feb, 2024 2 commits
 - add meta data
David Zimmer authored 1 day ago
b398fa41
 - Initial Structure and data
David Zimmer authored 2 days ago
ca13e345
- 15 Feb, 2024 1 commit
 - Initial Commit
David Zimmer authored 6 days ago
432ec2c6

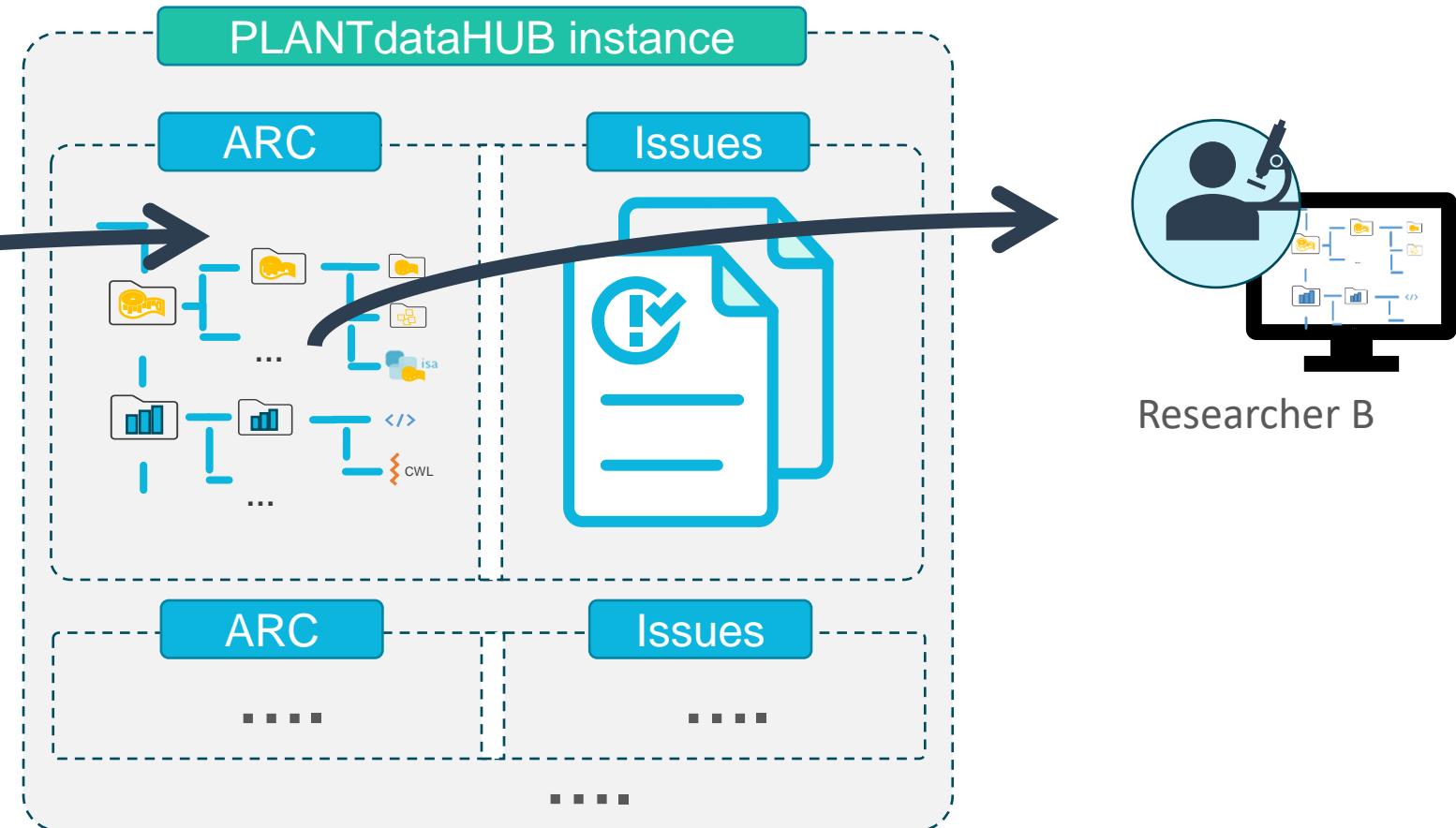
Below the commits, there is a "Search by message" input field and a "Author" dropdown.

Researcher A

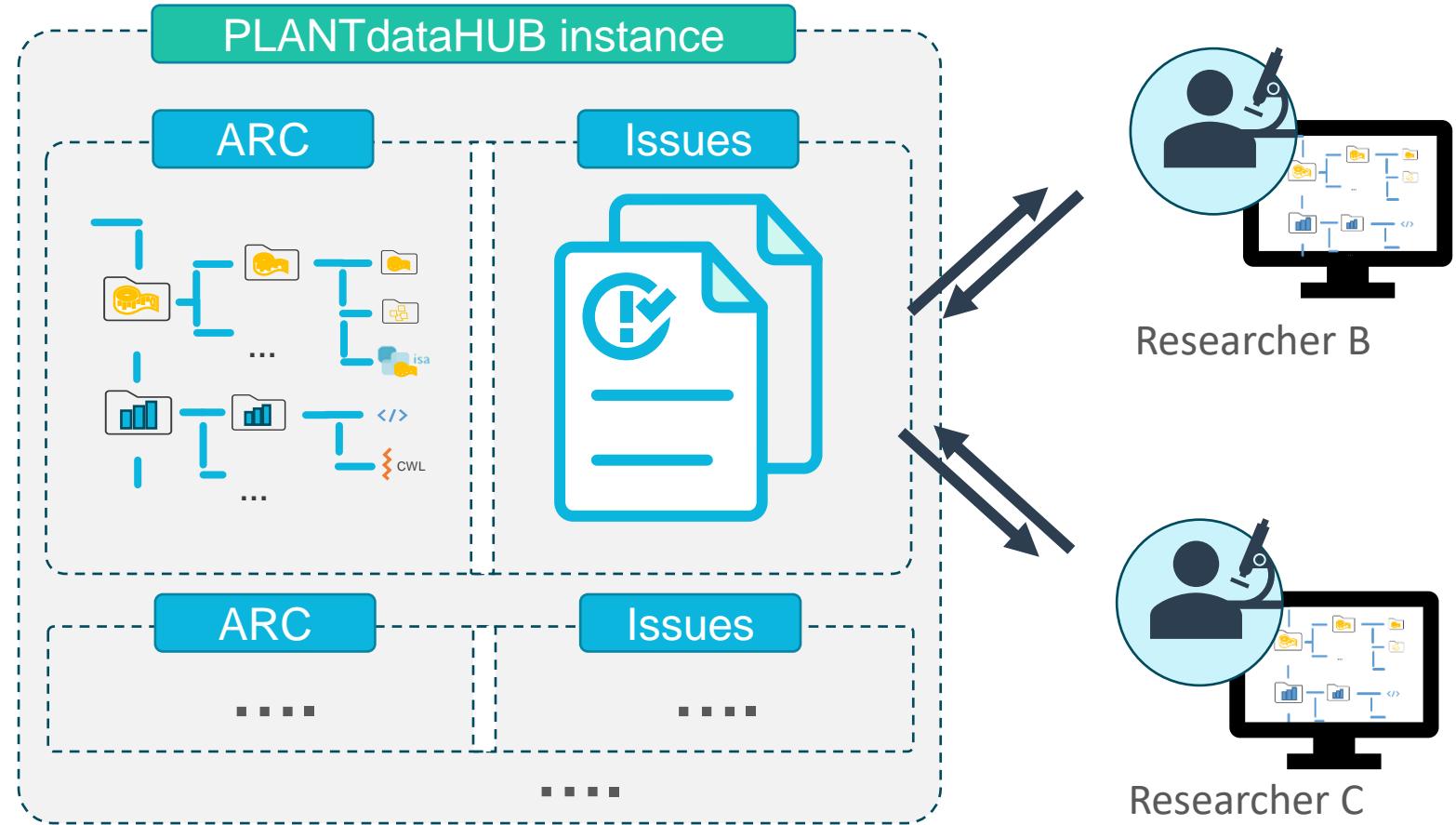
Now: Using the PLANTDataHUB to collaborate



Researcher A



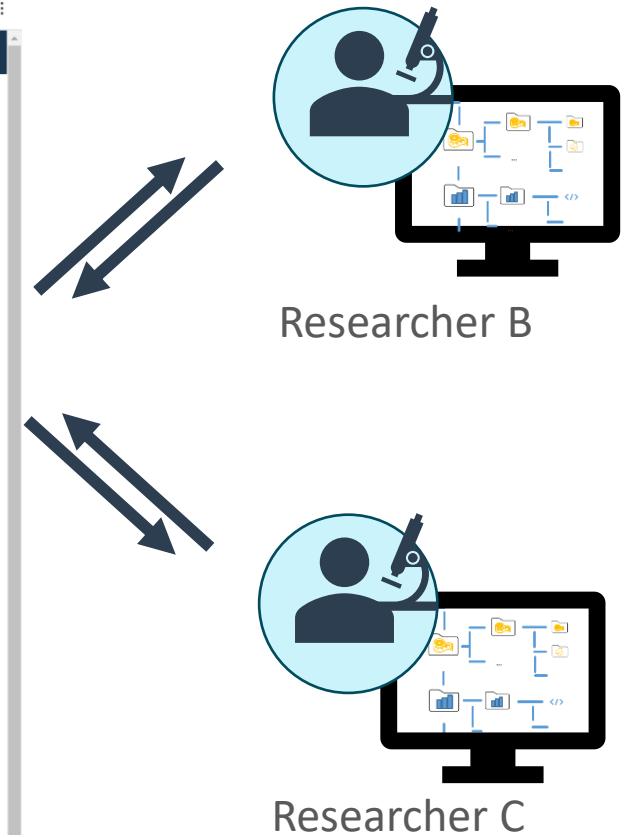
Now: Using the PLANTDataHUB to collaborate



Now: Using the PLANTDataHUB to collaborate

The screenshot shows the GitLab interface for the 'TurbolDWorkshop' project. The left sidebar contains navigation links like Project information, Repository, Issues, Merge requests, CI/CD, Security & Compliance, Deployments, Packages and registries, Infrastructure, Monitor, Analytics, Wiki, Snippets, and Settings. The main area displays project details: Project ID: 1079, 7 Commits, 1 Branch, 0 Tags, 40.4 MB Project Storage. A recent commit titled 'update analysis' by David Zimmer is shown, dated 19 hours ago. Below the commit is a file list with their last update times:

Name	Last commit	Last update
assays	update analysis	19 hours ago
runs	update analysis	19 hours ago
studies	update analysis	19 hours ago
workflows	add executable Workflow	22 hours ago
.gitattributes	update analysis	19 hours ago
.gitignore	Initial Commit	6 days ago
isa.investigation.xlsx	update analysis	19 hours ago

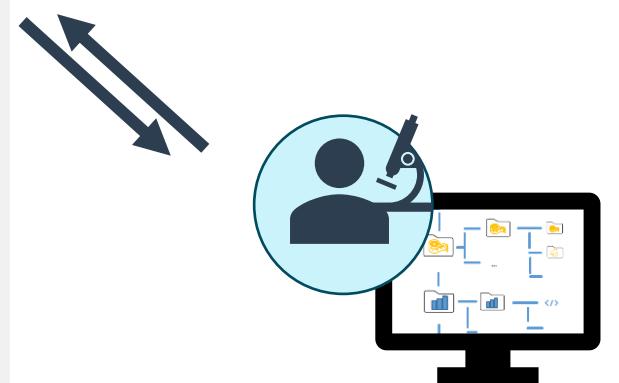


Now: Using the PLANTDataHUB to collaborate

The screenshot shows a GitLab interface for the project 'TurboIDWorkshop'. The left sidebar includes options like Project information, Repository, Issues (with 2 notifications), Boards, Service Desk, Milestones, Merge requests (0 notifications), CI/CD, Security & Compliance, Deployments, Packages and registries, Infrastructure, Monitor, Analytics, Wiki, Snippets, and Settings. The main area displays an 'Issues' page with three items: 'Ideas for complementary experiments' (3 issues), 'Add Information about medium in the study "Growth"' (1 issue), and another unnamed issue (1 issue). The issue 'Add Information about medium in the study "Growth"' is highlighted with a blue border.



Researcher B



Researcher C

Now: Using the PLANTDataHUB to collaborate

The screenshot shows a GitLab issue page for a project named 'TurboIDWorkshop'. The issue, created by David Zimmer, asks for information about a medium in a study titled 'Growth'. The interface includes a file upload area for designs, a task list with two items ('Download ARC' and 'Add missing information using the ARCIctect'), and an activity feed showing interactions between Heinrich Lukas Weil and David Zimmer.

Add Information about medium in the study "Growth"

I need this information to process the data can you please add this?

Drag your designs here or click to upload.

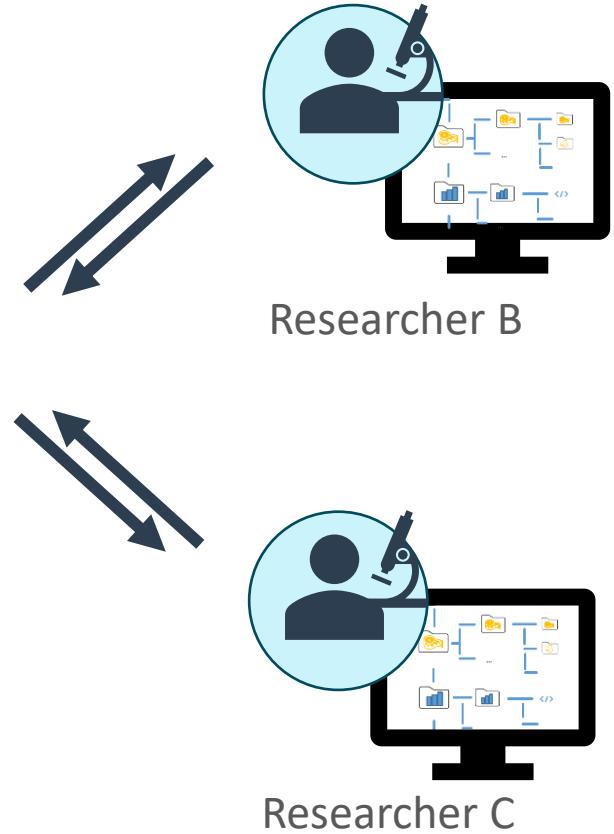
Tasks

- Download ARC
- Add missing information using the ARCIctect

Activity

Heinrich Lukas Weil @weil · 1 hour ago
Yeah sure, will look into it and add the information.

David Zimmer @zimmer · 1 minute ago
Great thank you!



Now: Using the PLANTDataHUB to collaborate

The screenshot shows a GitLab issue page for a project named 'TurboIDWorkshop'. The issue, created by David Zimmer, asks for information about a medium in a study titled 'Growth'. The page includes a 'Designs' section with a file upload area, a 'Tasks' section with two items: 'Download ARC' and 'Add missing information using the ARCIctect', and an 'Activity' section showing interactions between Heinrich Lukas Weil and David Zimmer.

Add Information about medium in the study "Growth"

I need this information to process the data can you please add this?

Designs Showing latest version

Drag your designs here or click to upload.

Tasks

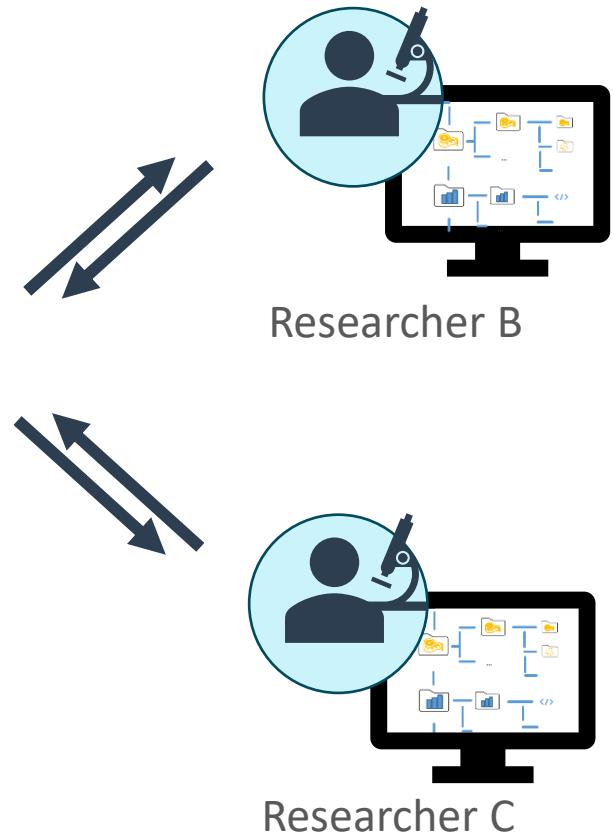
Download ARC

Add missing information using the ARCIctect

Activity

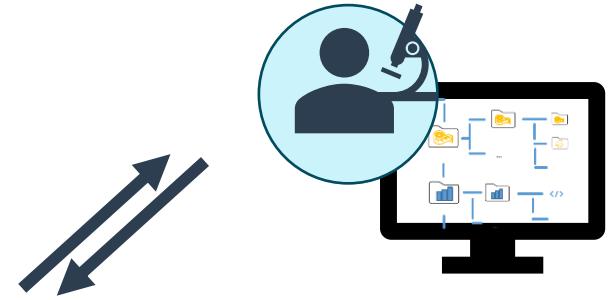
Heinrich Lukas Weil @weil · 1 hour ago
Yeah sure, will look into it and add the information.

David Zimmer @zimmer · 1 minute ago
Great thank you!

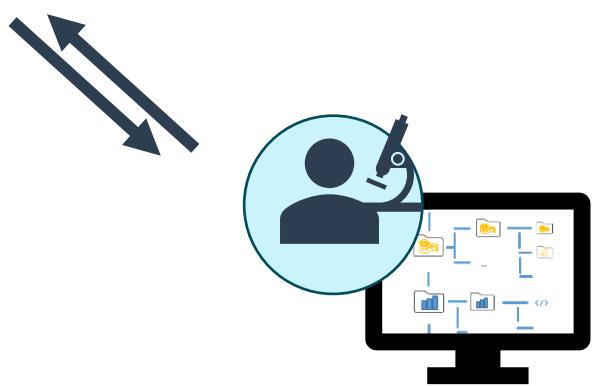


Now: Using the PLANTDataHUB to collaborate

The screenshot shows a web browser window displaying a GitLab project titled 'TurbоДWorkshop'. The left sidebar is a navigation menu with various options like 'Project information', 'Repository', 'Issues', 'Bugs', 'Merge requests', 'CI/CD', 'Security & Compliance', 'Deployments', 'Packages and registries', 'Infrastructure', 'Monitor', 'Analytics', 'Wiki', 'Snippets', and 'Settings'. The 'Milestones' option is currently selected and highlighted in blue. The main content area shows a 'Milestone' titled 'finalize first Version' with a Milestone ID of 9. It includes sections for 'Burndown Charts' (with a note about upgrading the license), 'Issues' (3 total, with 2 Unstarted, 0 Ongoing, and 1 Completed), and 'Merge requests' (0). Below these are three cards: 'Unstarted Issues (open and unassigned)' (2 items: 'Ideas for complementary experiments #3' and 'Add Information about medium in the study "Growth" #1'), 'Ongoing Issues (open and assigned)' (0), and 'Completed Issues (closed)' (1 item: 'Analysis request #2').

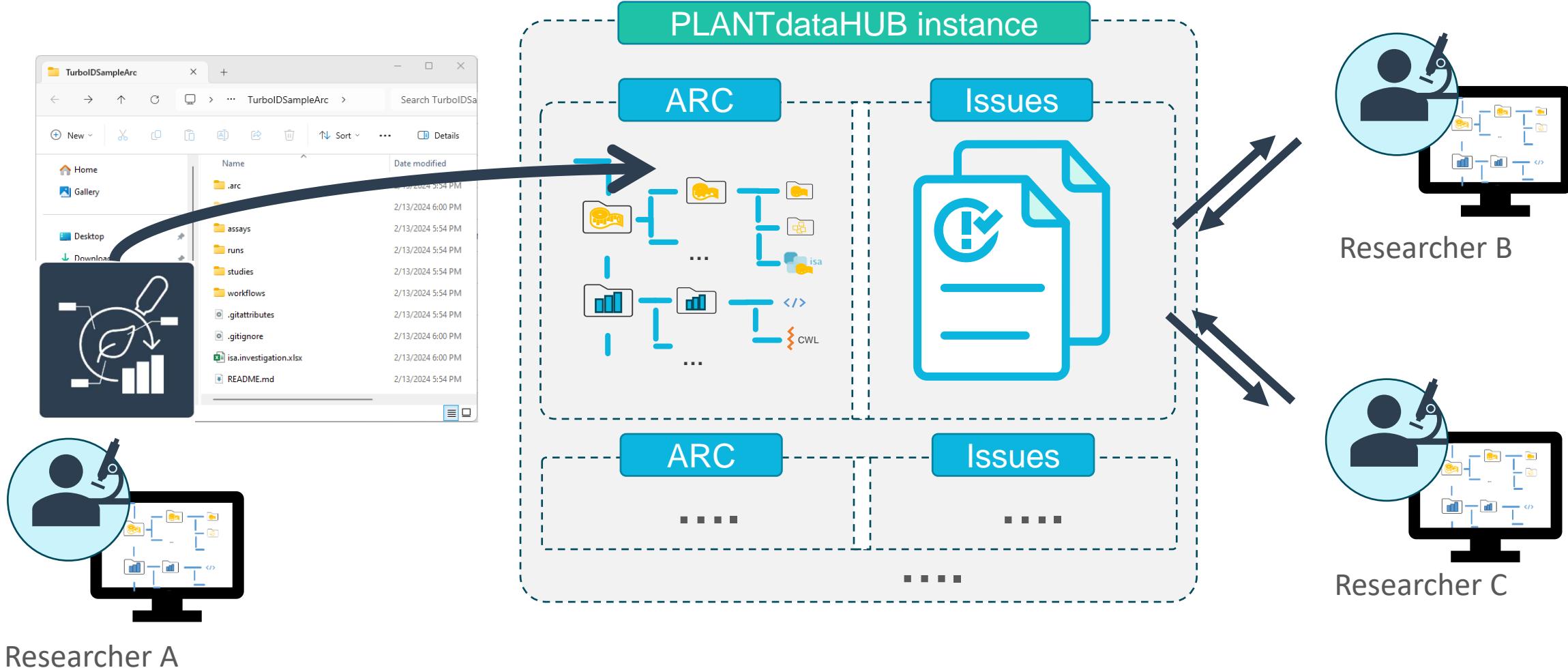


Researcher B



Researcher C

Now: Using the PLANTDataHUB to collaborate



Agenda of part two



- I. Important ARC concepts by example:
Structure
- II. Important ARC concepts by example:
Meta Data Annotation Principle
- III. ARCs for FAIR collaboration using the
PLANTDataHUB

IV. Complete Walk-Through
using the ARCitect



IV: Prerequisites

- Create an DataPLANT Account:
 - Visit: <https://git.nfdi4plants.org/explore>
 - Click “Sign in”
 - Either connect your ORCID account or create an DataPLANT account using “SIGN UP”
- Download the Arcitect:
 - This tutorial is performed using Arcitect version 0.0.28 newer versions might be available but might have an different look
 - The software is still at an early state, if you find bugs and want to help, please report your bugs [here](#)
- Optional: Have a look at the NFDI4Plants Knowledgebase

Agenda

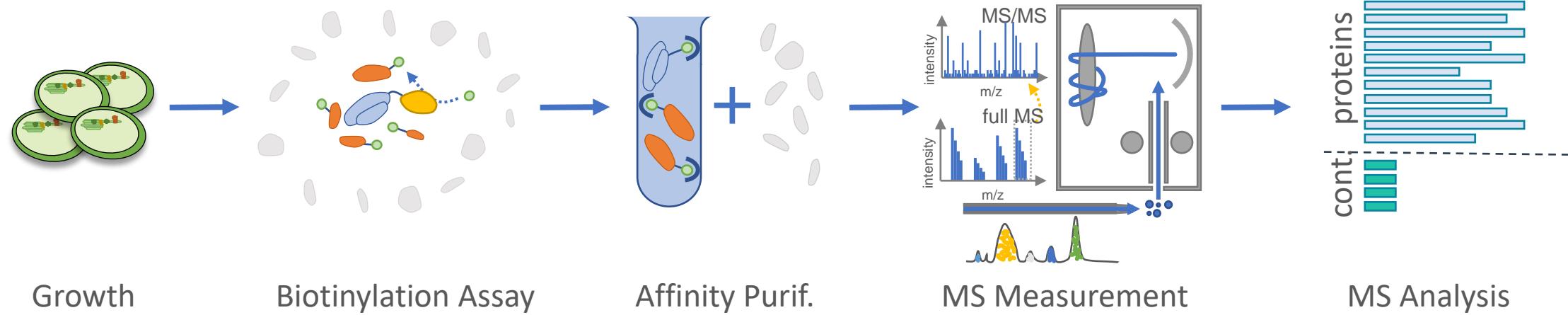
- I. Initialize ARC structure and add data
- II. Add Meta Data
- III. Login to the DataHUB and synchronize our ARC
- IV. Explore the ARC online
- V. Execute an workflow in the ARC

I. Initialize ARC structure and add data

- Open the Arcitect
- Create a new ARC

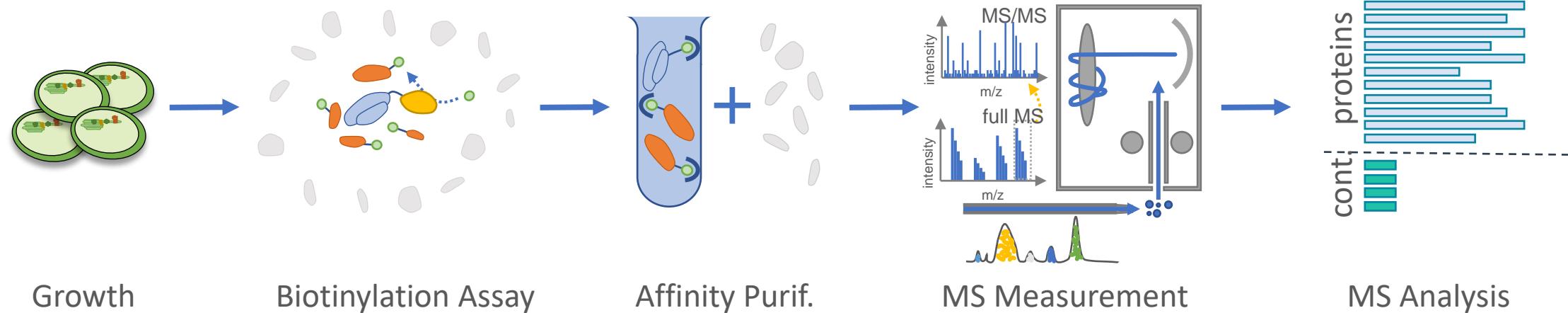
I. Initialize ARC structure and add data

- Inspect our experiment and layout the ARC accordingly
 - Add one study called growth



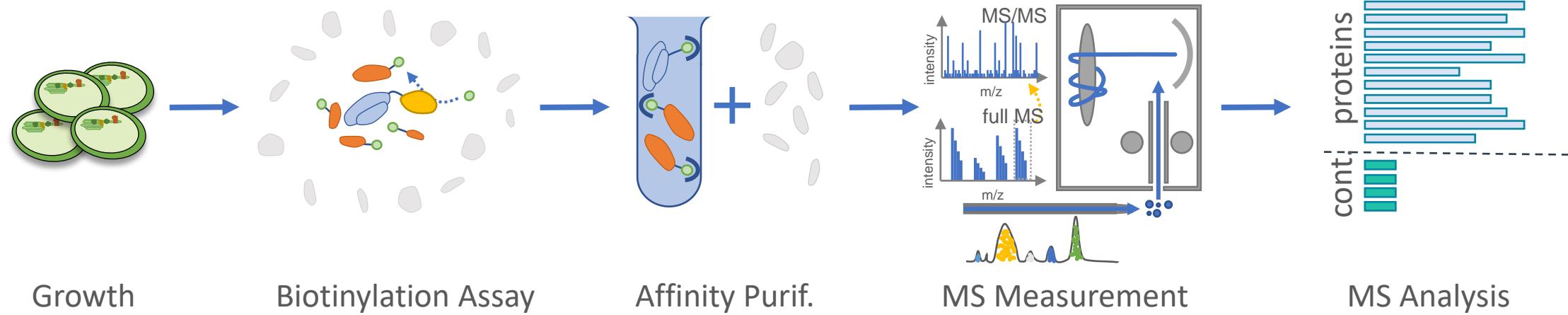
I. Initialize ARC structure and add data

- Inspect our experiment and layout the ARC accordingly
 - Add one study called growth
 - Add four Assays called “Biotinylation”, “AffinityPurification”, “MS Measurement” and “MS Analysis”



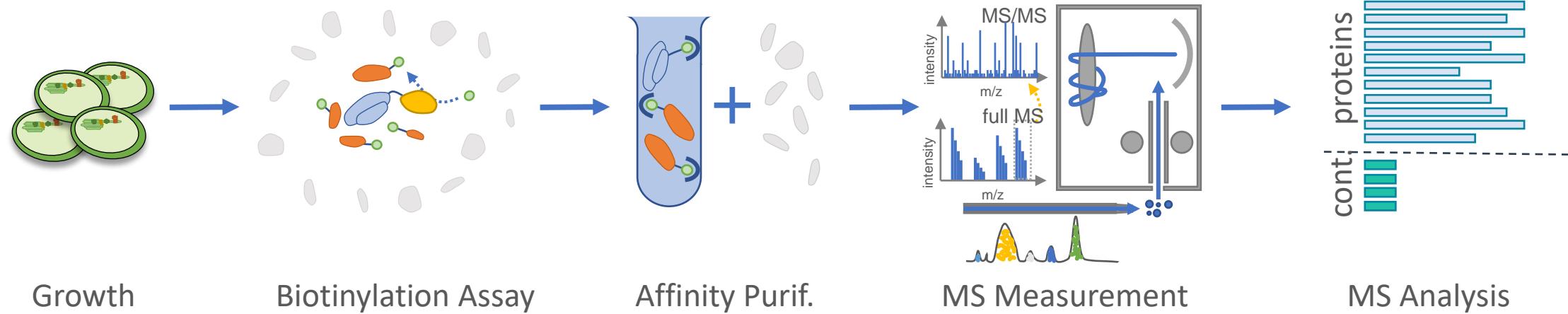
I. Initialize ARC structure and add data

- Add our experimental data
 - Add MS raw data to the assay `MSMeasurement`



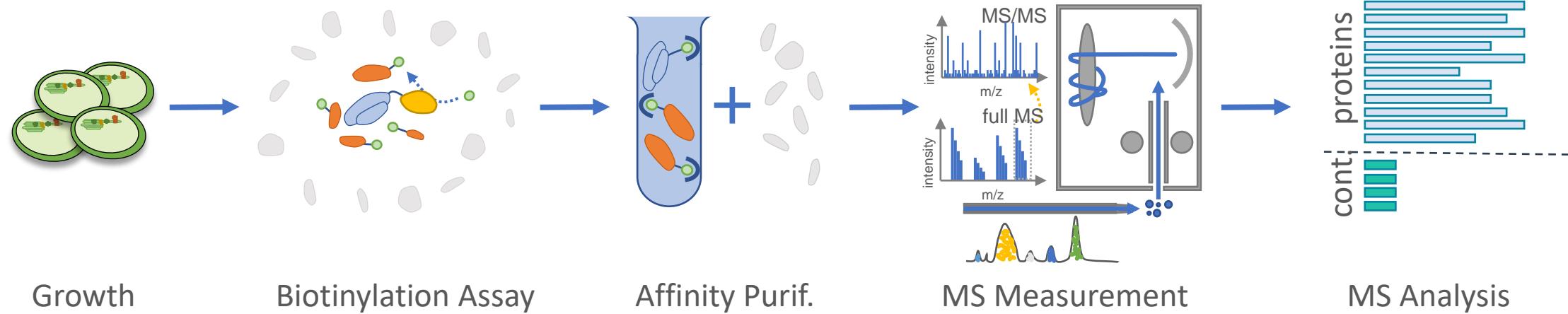
I. Initialize ARC structure and add data

- Add our experimental data
 - Add MS raw data to the assay `MSMeasurement`
 - Add MS analysis data to the `MSAnalysis` assay



I. Initialize ARC structure and add data

- Add our experimental data
 - Add MS raw data to the assay `MSMeasurement`
 - Add MS analysis data to the `MSAnalysis` assay



Agenda

- I. Initialize ARC structure and add data
- II. Add Meta Data
- III. Login to the DataHUB and synchronize our ARC
- IV. Explore the ARC online
- V. Execute an workflow in the ARC

II. Add Meta Data

- Add Meta Data to the study “Growth”
 - Visit the Growth study and add a new workbook and name it “Growth”

II. Add Meta Data

- Add Meta Data to the study “Growth”
 - Visit the Growth study and add a new workbook and name it “Growth”
 - Add an Input [Source Name] column and an Output [Sample Name] column

II. Add Meta Data

- Add Meta Data to the study “Growth”
 - Visit the Growth study and add a new workbook and name it “Growth”
 - Add an Input [Source Name] column and an Output [Sample Name] column
 - Add your Sources named “RBCL”, “FBP” and “Cher4”, each three times

II. Add Meta Data

- Add Meta Data to the study “Growth”
 - Visit the Growth study and add a new workbook and name it “Growth”
 - Add an Input [Source Name] column and an Output [Sample Name] column
 - Add your Sources named “RBCL”, “FBP” and “Cher4”, each three times
 - Add your Samples named “RBCL_Turbold_1_preExp”, “RBCL_Turbold_2_preExp” etc.

II. Add Meta Data

- Add Meta Data to the study “Growth”
 - Visit the Growth study and add a new workbook and name it “Growth”
 - Add an Input [Source Name] column and an Output [Sample Name] column
 - Add your Sources named “RBCL”, “FBP” and “Cher4”, each three times
 - Add your Samples named “RBCL_TurboID_1_preExp”,
“RBCL_TurboID_2_preExp” etc.
 - Add the columns Characteristic [organism], and Characteristic [biological replicate group] to describe the input

II. Add Meta Data

- Add Meta Data to the study “Growth”
 - Visit the Growth study and add a new workbook and name it “Growth”
 - Add an Input [Source Name] column and an Output [Sample Name] column
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 - Add your Samples named “RBCL_TurboID_1_preExp”,
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 - Add an Input [Source Name] column and an Output [Sample Name] column
 - Add your Sources named “RBCL”, “FBP” and “Cher4”, each three times
 - Add your Samples named “RBCL_Turboid_1_preExp”, “RBCL_Turboid_2_preExp” etc.
 - Add the columns Characteristic [organism], Characteristic [plasmid] and Characteristic [biological replicate group] to describe the input
 - Add the columns Parameter [temperature], Parameter [light intensity exposure] and Parameter [Biological replicate] to describe the process that produced our samples in the output column

II. Add Meta Data

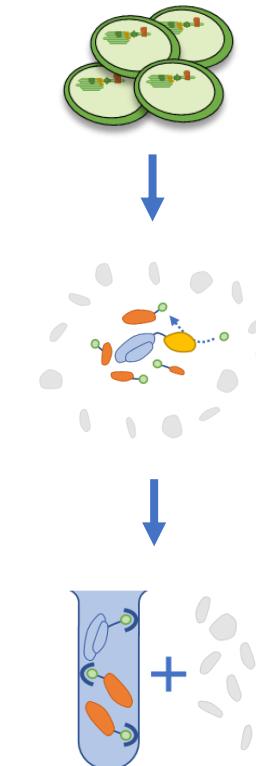
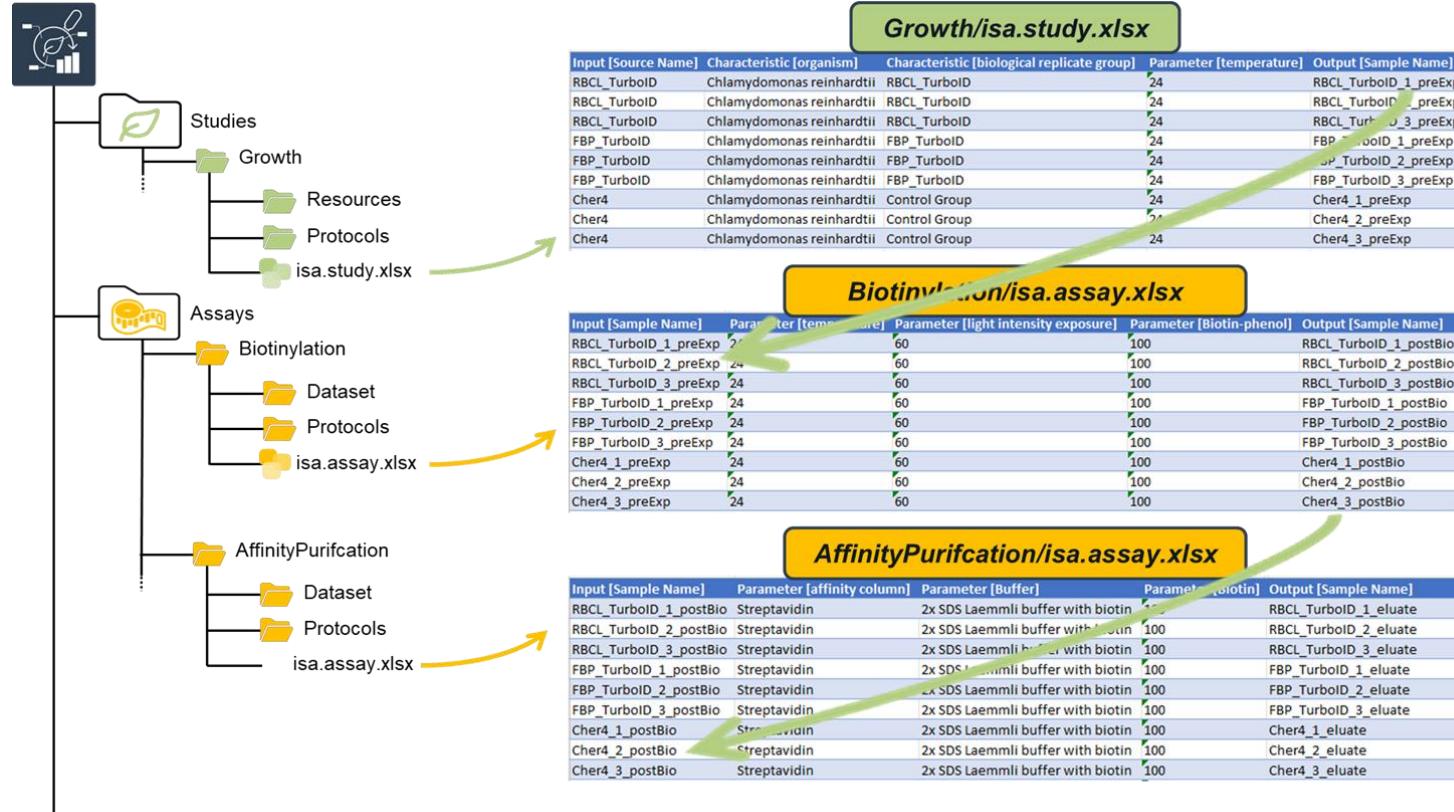
- Add Meta Data to the study “Growth”
 - Visit the Growth study and add a new workbook and name it “Growth”
 - Add an Input [Source Name] column and an Output [Sample Name] column
 - Add your Sources named “RBCL”, “FBP” and “Cher4”, each three times
 - Add your Samples named “RBCL_Turboid_1_preExp”, “RBCL_Turboid_2_preExp” etc.
 - Add the columns Characteristic [organism], Characteristic [plasmid] and Characteristic [biological replicate group] to describe the input
 - Add the columns Parameter [temperature], Parameter [light intensity exposure] and Parameter [Biological replicate] to describe the process that produced our samples in the output column

II. Add Meta Data

- Add Meta Data to the assay “Biotinylation”
- Visit the Assay “Biotinylation” and add a new workbook and name it “Biotinylation”
- Add an Input [Source Name] Column and Output [Sample Name] Column

II. Add Meta Data

- Add Meta Data to the assay “Biotinylation”



II. Add Meta Data

- Add Meta Data to the assay “Biotinylation”
- Visit the Assay “Biotinylation” and add a new workbook and name it “Biotinylation”

II. Add Meta Data

- Add Meta Data to the assay “Biotinylation”
- Visit the Assay “Biotinylation” and add a new workbook and name it “Biotinylation”
- Add Meta Data!

II. Add Meta Data

- Repeat for all assays
- ... or inspect the prepared ARC called “LiveARC_WithMetaData”

II. Add Meta Data

- Repeat for all assays
- ... or inspect the prepared ARC called “LiveARC_WithMetaData”
- Use the file picker to add file references to assays

II. Add Meta Data

- Repeat for all assays
- ... or inspect the prepared ARC called “LiveARC_WithMetaData”
- Use the file picker to add file references to assays
- Inspect the Output of the assay “AffinityPurification” and how it maps to the assay “Western Plot”

Agenda

- I. Initialize ARC structure and add data
- II. Add Meta Data
- III. Login to the DataHUB and synchronize our ARC
- IV. Explore the ARC online
- V. Execute an workflow in the ARC

III. Login to the DataHUB and synchronize our ARC

- Login to your DataPLANT account
- Commit our changes locally
- Sync our new Commit with the DataHUB

Agenda

- I. Initialize ARC structure and add data
- II. Add Meta Data
- III. Login to the DataHUB and synchronize our ARC
- IV. Explore the ARC online
- V. Execute an workflow in the ARC

IV. Explore the ARC online

- Visit the DataHUB and identify your ARC
- Explore your ARC structure
- Inspect your Commits

IV. Explore the ARC online

- Visit the DataHUB and identify your ARC
- Explore your ARC structure
- Inspect your Commits
- Make local changes and sync again
- Inspect your Commits

IV. Explore the ARC online

- Visit the DataHUB and identify your ARC
- Explore your ARC structure
- Inspect your Commits
- Make local changes and sync again
- Inspect your Commits
- Create an issue
- Create an milestone

Agenda

- I. Initialize ARC structure and add data
- II. Add Meta Data
- III. Login to the DataHUB and synchronize our ARC
- IV. Explore the ARC online
- V. Execute an workflow in the ARC

V. Execute an workflow in the ARC

- Add the workflow and the run parameters using the ARCitect
- Execute the workflow using cwltool as described [here](#)