

Hands-on Basic Training



Data publishing and archival at FAIRDOMhub

Alexey Kolodkin and Olga Krebs

ELIXIR-DMP-DS-training

“Best practices in research data management and stewardship”

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Preparing data for publications, and generating DOI

Task

You will be taught how to manage your data, from organising it in the FAIRDOMHub, through to publishing it ready for citation, and/or for inclusion in publications.



Expected Outcomes

- Being familiar with the ISA structure
- Setting up a full ISA structure with attached data and models.
- Making the ISA structure publicly available.
- Snapshotting the ISA and associated data and models.
- Assigning DOIs.

Pre-task



- Go to the sandbox instance set for training
<https://sandbox7.fairdomhub.org/>
- Log in with username/password for guests as listed in this document
- https://docs.google.com/spreadsheets/d/1gcaAtk2T9W1erdU0OkzISdjS_DPz1uG_ZF_3p4sZyM4/edit#gid=1137063622
- Your project
<https://sandbox7.fairdomhub.org/projects/9>
- Go to <https://sandbox7.fairdomhub.org/events/2>, look for associated Presentations and Hands-On-Instructions

Pre-task (continued)



For example data we will use <https://fairdomhub.org/>
(without login, data is publicly available)

Here you can find user guide and Help documents
<http://docs.seek4science.org/help/>

FAIRDOMHub: Landing page

The screenshot shows the FAIRDOMHub landing page. The top navigation bar includes the FAIRDOM logo, a search bar, and several menu items: 'Browse', 'Create', and 'Help'. A red arrow originates from the 'Help' menu item in the top navigation bar and points to a detailed help menu on the right side of the page. This detailed menu lists various support resources: 'Help', 'Help documents', 'Feedback', and 'Provide feedback'. Another red arrow points from the 'Create' menu item in the top navigation bar to a list of content types in the center-right area, including 'Assets', 'Data file', 'Model', 'SOP', 'Publication', 'Experiments', 'Investigation', 'Study', 'Assay', 'Activities', 'Presentation', 'Event', 'Admin', 'Programme', 'Project', 'Institution', and 'Profile'. The main content area features a large heading 'FAIRDOMHub' and introductory text about the initiative, which is partially obscured by the red arrows. On the left side, there are sections for 'Yellow pages' (listing categories like Programmes, People, Projects, etc.) and 'FAIRDOM News' (with recent updates).

Instructions



In the hands-on session you can either

- (i) use your own data, SOPs, to set up an ISA structure in SEEK
- (ii) use examples from FAIRDOMHub (e.g. templates with example data, SOPs, available to you)

Please note that the assets you create in a training sandbox instance will be available for the duration of the workshop (+ one month) and deleted afterwards

Research outcomes organised in an ISA (Investigation, Study, Assay/Analysis) format.



FAIRDOM Browse - Help - Search here... Search

Home / Investigations Index / Glucose metabolism in Plasmodium falciparum trophozoites

Glucose metabolism in Plasmodium falciparum trophozoites

The investigation entails the construction and validation of a detailed mathematical model for glycolysis of the malaria parasite Plasmodium falciparum in the blood stage trophozoite form.

ID-56

Projects: Whole body modelling of glucose metabolism in malaria patients

Selected item: Investigation: Glucose metabolism in Plasmodium falciparum trophozoites [Full graph \(9\)](#)

Investigation

Investigation: Glucose metabolism in Plasmodium falciparum trophozoites

Study

- Study: Model construction
- Study: Model validation
- Study: Model analysis
- Publication: Construction and validation of a detailed kinetic model of glycolysis in Plasmod...

Analysis (Assay)

Modelling Analysis: PFK

Related Items

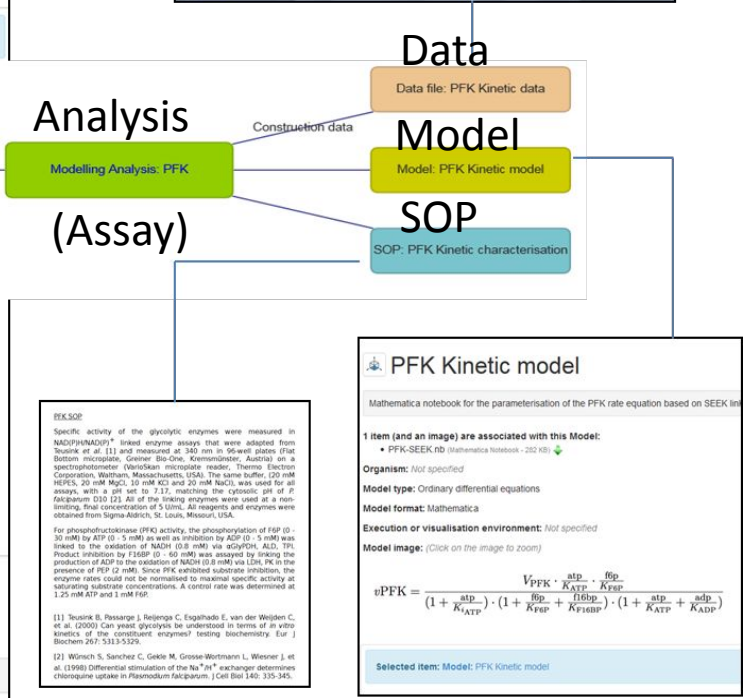
People (1) Projects (1) Studies (3) Assays (24) Data files (16) Models (19) SOPs (13) Publications (1)

David Van Niekerk

Projects: SysMO DB, Whole body modelling of glucose metabolism in malaria patients
Institutions: University of Stellenbosch

Disciplines: Modeller
Roles: Not specified
Expertise: Not specified
Tools: Not specified

Metadata	Values (examples)
Assay Title	PFK Kinetic Data
Uploader	Deves van Niekerk
Uploader SEEK ID	
Project	
ASSAY	
Assay SEEK ID	0
Assay Title	PFK Kinetic Assay
Assay Type	Microplate Assay
Technology Type	well-plate experiment
Description	Kinetic characterisation of PFK, Export
Experimentation	Great Protein
Date	
DOI	
Publication (optional)	
Experimental_conditions	
Time	
Component (of concentration)	temperature pH Buffer Buffer Buffer Buffer
Unit	HEPES MgCl2 KCl Suc2
Value	mM mM mM mM
Start_value (optional)	7.17 20 10 10 20
End_value (optional)	
Comments	
Other growth	Block
FACTORS_STUDIED	
Item	concentration concentration concentration concentration
Component (of concentration)	ATP F6P
Unit	mM mM mM mM
Value	0.214715 0 0 0
Start_value (optional)	10 5 5 40
End_value (optional)	
Comments	



Tasks



- **T1.** Creating and interlinking ISA elements
- **T2.** Downloading spreadsheet templates-based data from SEEK, editing it and uploading to own ASSAY created in T1.
- **T3.** Creating SOP (as link to Nature protocols) spreadsheet templates for the semantic annotation of data, link it to data file
- **T4.** Registering publications (with DOI or PubmedID), linking it to ISA, data file.
- **T5.** Create model, upload image representing e.g. pathway your model describes
- **T5.** Publishing your data in FAIRDOMHub
- *T6. (optional) Creating/using sample types and (bio)samples*

Task 1. Creating new ISA











- Go to pre-created Investigation <https://sandbox7.fairdomhub.org/investigations/4>, associated it to your project or create your own **Investigation**
- Add a new **Study**, associate it to your project, share it with your project
- Scroll down to the I-S-A graph, navigate to the **Study** page
- Add new **experimental Assay** to the **Study** created
- Define assay type and appropriate technology type (choose from the drop-down lists)
- Assign your **Assay** to the existing **Study**
- Define the access rights for your **Assay** – e.g. sharing it with own project, or with single person
-


Access Permissions : Just Enough Sharing


Sharing ▲

Here you can specify who can **view** the summary of and **edit** the Investigation.

	No Access	View	Edit	Manage	
 Public	<input checked="" type="checkbox"/>	<input type="checkbox"/>			
 Best practices in FAIR data management and stewardship	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	
 Alexey Kolodkin	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	✕
 Xiaoming Hu	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	✕
 Teacher1 Profile	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	✕

 Share with a person

 Share with a project/institution

 Share with a programme

Task 1a. Creating new ISA



- Navigate back to the **Study** page (via menü or using I-S-A graph)
- Add new **modelling analysis Assay** to your **Study**
- Define **Model type , Model format, and Preferred execution or visualisation environment** (choose from the drop-down lists)
- Assign your **Assay** to the existing **Study**
- Define the access rights for your **Assay** – e.g. sharing it with own project, or with single person

Task 2. 1 Downloading and uploading data



- Go to https://fairdomhub.org/data_files/927/ to get a data example file **(or use your own data file)**
- Visualise data content, look for spreadsheet structure and format
- Download this **data file** and open it
- Fill in some reasonable example data. This spreadsheet has been created using RightField, so you can select values from the drop-down lists in the spreadsheet
- Save the **data file** with a new name on your PC
- Upload (create new **data file**) **this file** to <https://sandbox7.fairdomhub.org/>
- Describe your data
- Link the data file to own experimental **assay** created in T1.

Task 2.2 Sharing data file



- Share **data file** with (i) project (ii) certain person (iii) public
- Define a temporary public link to your **data file** (expiring e.g. at end of October 2020)
- Logout and check whether you can access the **file** directly via **temporary URL**
- Subsequently make the **file** public
- Logout and check whether you can find and access the **data file** by browsing

Task 3. Creating SOP



- Go to example **SOP** <https://fairdomhub.org/sops/253> to get an example SOP or Go to Nature protocol exchange page and choose any protocol (e.g. <http://www.nature.com/protocolexchange/protocols/4761>)
or use your own local SOP file
- Go to FAIRDOMHub , create new SOP as
 - a) external link to Nature protocols (URL)
 - b) upload local file (downloaded from FAIRDOMHub or your own prepared SOP)
- Share it with own project, or with single person
- Link **SOP** to experimental **Assay** created in T1.

Task 4. Registering publications



- Go to Pubmed and choose any publication of your interest, copy PubmedID
- Go to FAIRDOMHub and register new **Publication** (using PubmedID or DOI)
 - select **Publication** from Create menu
 - choose PubMed ID or DOI – insert the corresponding ID, click “Fetch” button
 - confirm abstract and authors list, finish
- Link **publication** to **Assay** created in T1.

Task 5 Create model, upload image representing e.g. pathway your model describes



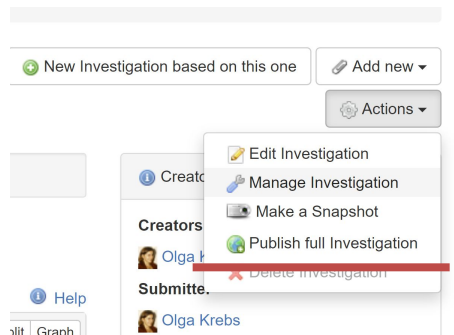
- Go to Biomodels Database choose e.g. <https://www.ebi.ac.uk/biomodels/BIOMD0000000502#Overview>, download SBML file
- Go to your modelling Assay in sandbox7 , choose “add new model” , fill in required fields
- Define image file for this model
- List creators’ names

Task 6. Publish your data via FAIRDOMHub

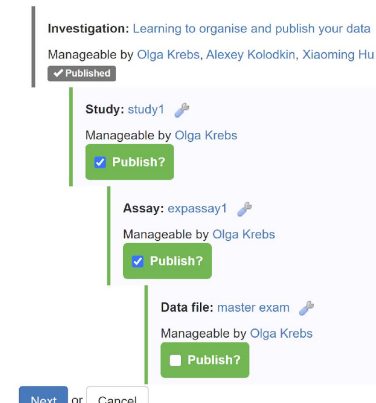


- Go to your Investigation

<https://sandbox7.fairdomhub.org/investigations/4> and open „Actions“ menu, choose „Publish full investigation“ option



If you have the required access rights, you can choose to publish it disabled. Somebody that can publish that item is listed next to it ar



- Create a snapshot
- Create DOI (*this does not work in sandbox, of course, because there are no toy-or test- DOIs*), here live example of DOI for ISA used as supplementary material for published paper <https://fairdomhub.org/investigations/74>

Live version of Experiment Linked to Journals

<https://fairdomhub.org/investigations/74>



Metabolic analysis of effects of sucrose translocation on phenotypic traits of *Arabidopsis thaliana*

Sucrose translocation between plant tissues is crucial for growth, development and reproduction of plants. Systemic analysis of this metabolic underlying regulatory processes can help to achieve better understanding of carbon distribution within the plant and the formation of phenotypic traits. Sucrose translocation from 'source' tissues (e.g. mesophyll) to 'sink' tissues (e.g. root) is tightly bound to the proton gradient across the membranes. Transporters are grouped into efflux exporters (SWEET family) and proton-symport importers (SUC, STP families). To better understand the connections between sucrose export from source tissues and sucrose import into sink tissues, there is a need for a metabolic model that takes into account the tissue organisation of *Arabidopsis thaliana* with corresponding metabolic specificities of respective tissues in terms of sucrose and proton proton transport. An ability of the model to operate under different light modes ('light' and 'dark') and correspondingly in different energy producing modes is also a feature.

 **BMC** Part of Springer Nature

BMC Plant Biology

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Research article | [Open Access](#) | Published: 28 December 2016

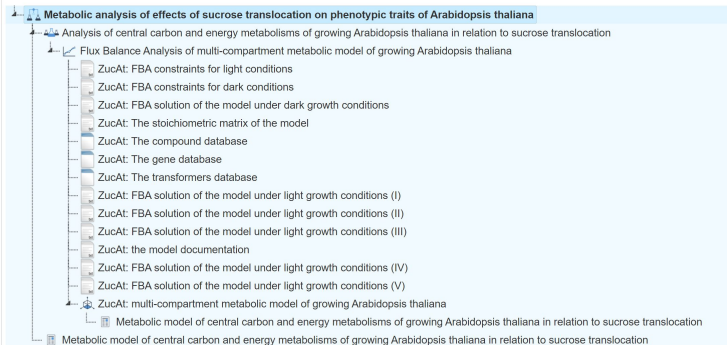
Metabolic model of central carbon and energy metabolisms of growing *Arabidopsis thaliana* in relation to sucrose translocation

[Maksim Zakhartsev](#), [Irina Medvedeva](#), [Yury Orlov](#), [Ilya Akberdin](#), [Olga Krebs](#) & [Waltraud X. Schulze](#) 

BMC Plant Biology **16**, Article number: 262 (2016) | [Cite this article](#)

3107 Accesses | 13 Citations | [Metrics](#)

Selected: Metabolic analysis of effects of sucrose translocation on phenotypic traits of *Arabidopsis thaliana* (Investigation)
Description: Sucrose translocation between plant tissues is crucial for growth, development and reproduction of plants. Systemic...
SEEK ID: <https://fairdomhub.org/investigations/74>



Snapshots

Snapshot 9 (4th Jun 2016) 
Snapshot 8 (25th Apr 2016) 

Activity

Views: 3822

Created: 21st Dec 2015 at 14:12
Last updated: 24th Apr 2016 at 11:04



Task 6. Open/ Edit /Create sample type



Created by Happy Salmon Co. for describing Library prep of RNA samples from Salmon.

Template

Template Feed Switch Library Prep.xlsx - [Download](#)

Attributes

- Sample Origin ID (String) *
- *Sample Origin Name (SEEK Sample - Salmon Liver Tissue Sample) **
- Plate ID (String) *
- Position (String) *
- Index name (String) *
- Index Seq (String) *
- Qubit BR kit Conc. (ng/ul) (String)
- BioAnalyzer Conc. (ng/ul) (String)
- BioAnalyzer bp (region 200-1200) (String)



Task 5. 1 Open/ Edit /Create sample type



Tags

testing x samples club x example x food x cooking x

Attributes

Re-arrange attributes by clicking and dragging the button on the left-hand side of each row.

Order	Name	Required?	Title?	Type	Unit	
↕ 1	Bake ID	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	String		Remove
↕ 2	Date of bake	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Date time		Remove
↕ 3	Cooking temperature	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Float	°C	Remove
↕ 4	Cooking time	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Integer	min minute	Remove
↕ 5	Type of Apple	<input type="checkbox"/>	<input type="checkbox"/>	Controlled Vocabulary		Remove
				Apples		
				+ New		
↕ 6	Comments	<input type="checkbox"/>	<input type="checkbox"/>	Text		Remove
↕ 7	Picture of result	<input type="checkbox"/>	<input type="checkbox"/>	Web link		Remove

+ Add new attribute

New sample type in SEEK

Attributes

Re-arrange attributes by clicking and dragging the button on the left-hand side of each row.

Order	Name	Required?	Title?	Type	Unit
↑↓ 1	Sample ID or name	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	String	
↑↓ 2	Cell culture name	<input checked="" type="checkbox"/>	<input type="checkbox"/>	String	
↑↓ 3	Cell culture lab identifier	<input type="checkbox"/>	<input type="checkbox"/>	String	
↑↓ 4	Cell culture start date	<input type="checkbox"/>	<input type="checkbox"/>	Date	
↑↓ 5	Cell culture growth type	<input type="checkbox"/>	<input type="checkbox"/>	Controlled Vocabulary SysMO Cell Culture Growth Type	
↑↓ 6	Cell culture comment	<input type="checkbox"/>	<input type="checkbox"/>	Text	
↑↓ 7	Cell culture provider name	<input type="checkbox"/>	<input type="checkbox"/>	String	
↑↓ 8	Cell culture provider identifier	<input type="checkbox"/>	<input type="checkbox"/>	String	Remove
↑↓ 9	Cell culture strain	<input checked="" type="checkbox"/>	<input type="checkbox"/>	SEEK Strain	