

Instructions to using SEEK to manage your research assets

Olga Krebs



Pre-task



- Pick up your assigned username/password (as sandbox guest) from “Working_Groups” file in google drive :
https://docs.google.com/spreadsheets/d/1KTCIX1xJdAg0ljjpXDbHoT6Dbue8kCPYp_HudIJU7bk/edit#gid=
- Go to the sandbox SEEK instance
<https://sandbox7.fairdomhub.org/>, log in
- All users are member of the project “Modelling COVID-19 epidemics” <https://sandbox7.fairdomhub.org/projects/9>
- Go to <https://sandbox7.fairdomhub.org/events/2>, look for Hands-On-Instructions linked to this Event or use Instructions stored in google drive course folder:
https://drive.google.com/drive/folders/1s0PU6q7V6p4SyVD8_5vgOG3QmuTpSgkO

Pre-task (continued)



We will use original data/model stored in FAIRDOMHub
<https://fairdomhub.org/investigations/372>
(without login, data is publicly available)

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



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

FAIRDOMHub: Landing page

The screenshot shows the FAIRDOMHub landing page. The top navigation bar includes the FAIRDOM logo, a search bar, and menu items for 'Browse', 'Create', and 'Help'. A red arrow points from the 'Help' menu item in the top bar to a larger 'Help' dropdown menu on the right side of the page. Another red arrow points from the 'Create' menu item in the top bar to a 'Create' dropdown menu on the right side of the page. The main content area features a 'FAIRDOMHub' header, a description of the initiative, and a list of categories such as 'Yellow pages', 'Programmes', 'People', 'Projects', 'Institutions', 'Experiments', 'Investigations', 'Studies', 'Assays', 'Assets', 'Data files', 'Models', 'SOPs', 'Publications', 'Activities', and 'Presentations'. A 'Community News' section is also visible at the bottom right of the main content area.

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:50

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...

Related Items

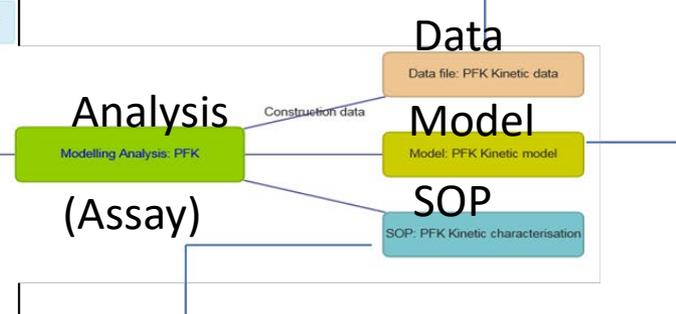
People (1) Projects (1) Studies (3) Assays (24) Data files (16) Models (19) SOPs (13) Publications (1)

David Van Niekirk

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

Disciplines: Molecular
Roles: Not specified
Expertise: Not specified
Tools: Not specified

Metadata		Values (example)			
Assay Title	PFK Kinetic Data				
Uploader	Deves van Niekirk				
Uploader SEEK ID					
Project					
ASSAY					
Assay SEEK ID	0				
Assay Title	PFK				
Assay Type	Microplate Assay				
Technique Type	Enzyme Assay				
Description	Kinetic characterisation of PFK, Enzyme				
Experimentation	Enzyme Assay				
DOI					
Publication (optional)					
Experimental_conditions					
Component (if concentration)	Temperature	pH	Buffer	Substrate	Buffer
Unit	°C		HEPES	MgCl ₂	KCl
Value	37	7.17	10	10	10
End_value (optional)			mM	mM	mM
Comments					
Culture growth	Batch				
FACTORS_STUDIED					
Item	Concentration	Concentration	Concentration	Concentration	
Component (if concentration)	ATP	ADP	FDP	F6P	
Unit	mM	mM	mM	mM	
Value	0.214717	0	0	0	
End_value (optional)	10	5	5	40	
Comments					



PFK SOP

Specific activity of the glycolytic enzymes were measured in NAD(P)H/NAD(P)⁺ linked enzyme assays that were adapted from Teukoll et al. [1] and measured at 360 nm in 96-well plates (Flat Bottom microplate, Greiner Bio-One, Kremsmünster, Austria) on a spectrophotometer (Microplate microplate reader, Thermo, Electron Corporation, Waltham, Massachusetts USA). The same buffer, (20 mM HEPES, 20 mM MgCl₂, 10 mM KCl and 20 mM sucrose) was used for all assays, with a pH set to 7.17, matching the cytosolic pH of *P. falciparum* [2]. All of the linking enzymes were used at a non-limiting, final concentration of 5 U/ml. All reagents and enzymes were obtained from Sigma-Aldrich, St. Louis, Missouri, USA.

For phosphofruktokinase (PFK) activity, the phosphorylation of FDP (0 - 30 mM) by ATP (0 - 5 mM) as well as inhibition by ADP (0 - 5 mM) was linked to the oxidation of NADH (0.8 mM) via acyl-P_i ADP. The product inhibition by F3BP (0 - 60 mM) was assayed by linking the production of ADP to the oxidation of NADH (0.8 mM) via LDH. PFK in the presence of FDP (2 mM). Since PFK exhibited substrate inhibition, the enzyme rates could not be normalised to maximal specific activity at saturating substrate concentrations. A control rate was determined at 1.25 mM ATP and 1 mM FDP.

[1] Teukoll B, Passarge J, Rejzinger C, Eggshahd E, van der Weijden C, et al. (2009) Can yeast glycolysis be understood in terms of in vitro kinetics of the constituent enzymes? testing biochemistry. Eur J Biochem 287: 5313-5320.

[2] Wörnisch S, Sanchez C, Gekle M, Grosse-Wilde M, Wiesner J, et al. (1998) Differential stimulation of the Na⁺/H⁺ exchanger determines chromosome uptake in Plasmodium falciparum. J Cell Biol 140: 335-345.

PFK Kinetic model

Mathematica notebook for the parameterisation of the PFK rate equation based on SEEK ID 50

1 item (an image) are associated with this Model:

- PFK-SEEK ID (Mathematica Notebook - 202 KB)

Organism: Not specified

Model type: Ordinary differential equations

Model format: Mathematica

Execution or visualisation environment: Not specified

Model image: (Click on the image to zoom)

$$v_{PFK} = \frac{V_{PFK} \cdot \frac{atp}{K_{ATP}} \cdot \frac{f6p}{K_{F6P}}}{\left(1 + \frac{atp}{K_{ATP}}\right) \cdot \left(1 + \frac{f6p}{K_{F6P}} + \frac{(f6p)^2}{K_{F6P}^2}\right) \cdot \left(1 + \frac{atp}{K_{ATP}} + \frac{atp}{K_{ADP}}\right)}$$

Selected item: Model: PFK Kinetic model

Tasks



- **T1.** Creating and interlinking ISA elements
- **T2.** Downloading data file from FAIRDOMHub, editing it and uploading to own ASSAY created in T1.
- **T3.** Creating SOP (as link to external repository)
- **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

Task 1. Creating new ISA



- Go to pre-created **Investigation** <https://sandbox7.fairdomhub.org/investigations/4> , associated it to your project
- 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 **modeling analysis Assay** to your **Study**
- Define **Model type , Model format, and Preferred execution or visualisation environment** (choose from the drop-down lists) 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 type="radio"/>			
 Best practices in FAIR data management and stewardship	<input type="radio"/>			<input type="radio"/>	
 Alexey Kolodkin	<input type="radio"/>				
 Xiaoming Hu	<input type="radio"/>				
 Teacher1 Profile	<input type="radio"/>			<input type="radio"/>	

 Share with a person

 Share with a project/institution

 Share with a programme

Task 2. 1 Downloading and uploading data



- Go to https://fairdomhub.org/data_files/3708 to get a data example file **(or use your own data file)**
- Visualise data content
- Download this **data file** and open it, 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 **modelling 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



- Create **SOP** as an external link to “Instructions for running the Corona Model of Westerhoff and Kolodkin on JWS Online” stored in FAIRDOMHub <https://fairdomhub.org/documents/670> to get an example SOP or **or use your own local SOP file**
- 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 (e.g. Kolodkin, Westerhoff paper)
- 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 your model



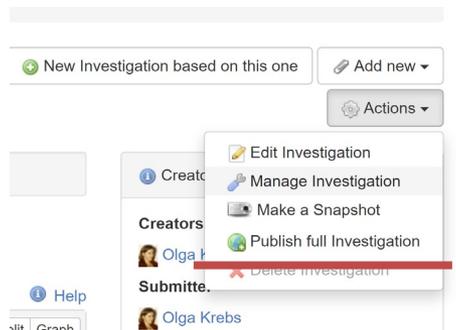
- Upload your **model**: go to your **modelling Assay** in sandbox7 , choose “add new model” , fill in required fields
- Define image file for this **model**
- List creators’ names
- Define sharing permissions

Task 6. Publish your data via FAIRDOMHub

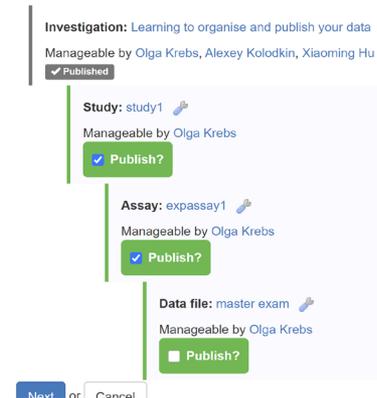


- Go to your Investigation

<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>

Task 7 – during and after this course : make your model representation **FAIR**



- upload all versions of your **model** (in SBML format)
- write and upload your own **SOP** about modeling process and steps
- Produce **data file** with simulation results, upload them as simulation results
- link all assets to your modeling **Assay**