Introduction to FAIRDOM-SEEK

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HITS Heidelberg Institute for Theoretical Studies

de.NBI GERMAN NETWORK FOR BIOINFORMATICS INFRASTRUCTURE

elixir

FAIRDOM

FAIRDOM Initiative

http://fair-dom.org

Findable
Accessible
Interoperable
Reusable

Data
Operations
Models

- develop a community
- establish an internationally sustained Data and Model Management service

FAIRDOM-SEEK Software

FAIRDOM SEEK

https://fairdomseek.org

- Open source web platform
- Storing, interlinking, sharing of scientific research data, models, protocols, publications etc. (no file format restrictions)
- Yellow pages with information about the people and organisations
- ISA (Investigation, Study, Assay) structure for describing how individual experiments are aggregated into studies and investigations
- Flexible and detailed sharing permissions
- DOI can be generated for individual items, or entire data sets

FAIRDOM-SEEK Software

Models

People

Data files
Documents

Samples

Programmes
Projects

Standard
Operating
Procedures

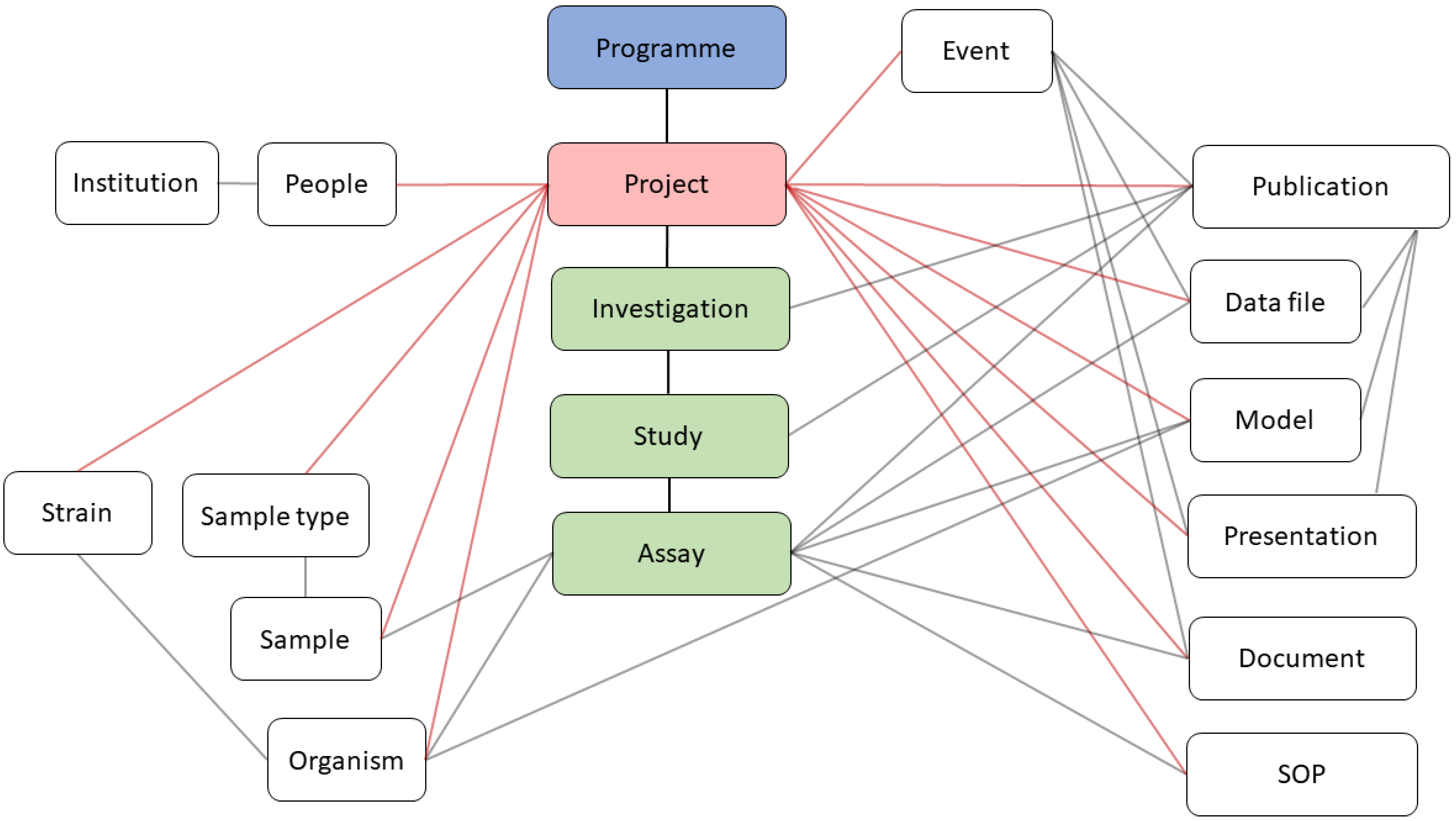
Publications

Events

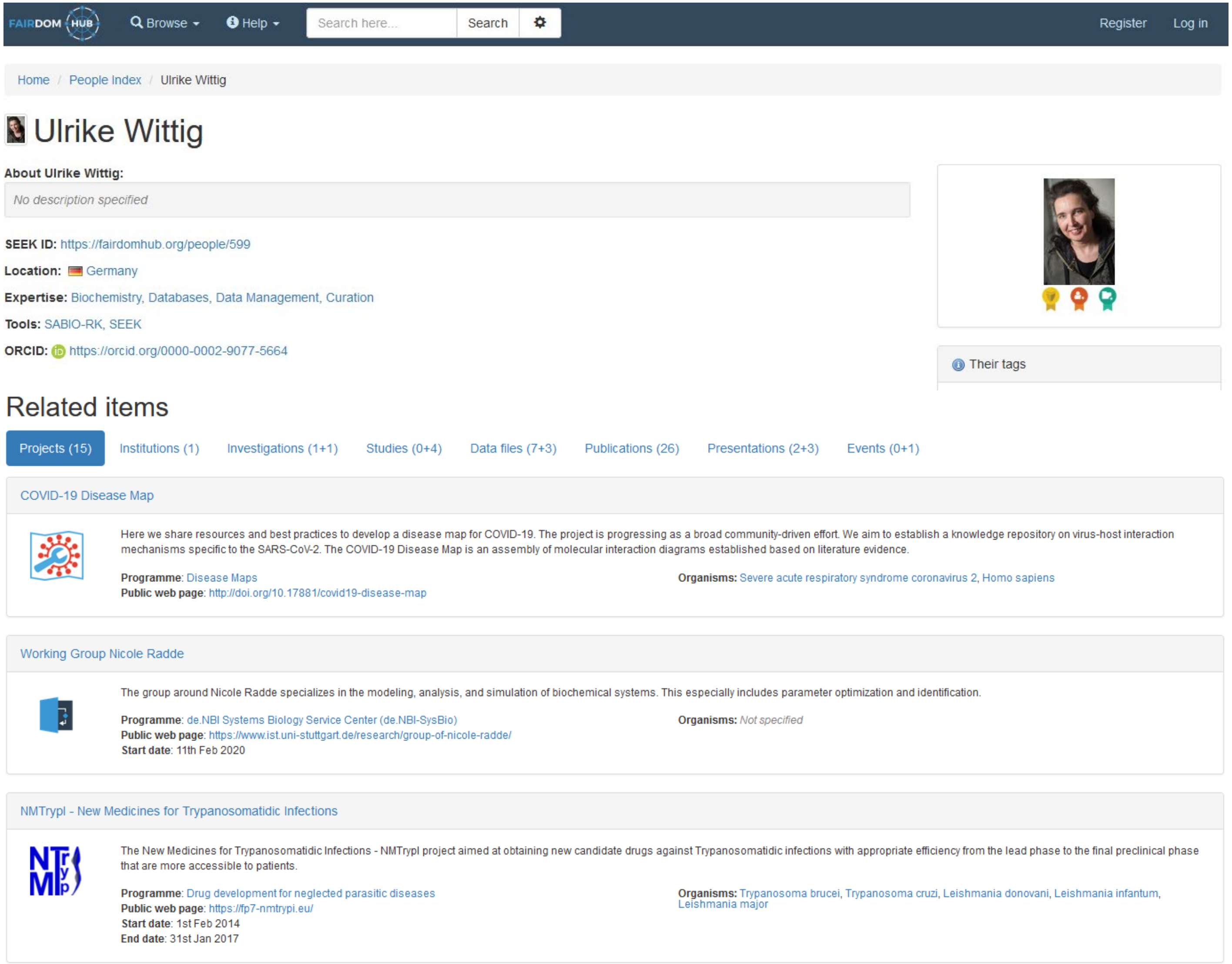
Presentations

Workflows

Programme - Project



People - Yellow Pages



Ulrike Wittig

About Ulrike Wittig:

No description specified

SEEK ID: https://fairdomhub.org/people/599

Location: Germany

Expertise: Biochemistry, Databases, Data Management, Curation

Tools: SABIO-RK, SEEK

ORCID: https://orcid.org/0000-0002-9077-5664

Related items

COVID-19 Disease Map

Here we share resources and best practices to develop a disease map for COVID-19. The project is progressing as a broad community-driven effort. We aim to establish a knowledge repository on virus-host interaction mechanisms specific to the SARS-CoV-2. The COVID-19 Disease Map is an assembly of molecular interaction diagrams established based on literature evidence.

Programme: Disease Maps
Public web page: http://doi.org/10.17881/covid19-disease-map
Organisms: Severe acute respiratory syndrome coronavirus 2, Homo sapiens

Working Group Nicole Radde

The group around Nicole Radde specializes in the modeling, analysis, and simulation of biochemical systems. This especially includes parameter optimization and identification.

Programme: de.NBI Systems Biology Service Center (de.NBI-SysBio)
Public web page: https://www.ist.uni-stuttgart.de/research/group-of-nicole-radde/
Start date: 11th Feb 2020
Organisms: *Not specified*

NMTrypI - New Medicines for Trypanosomatidic Infections

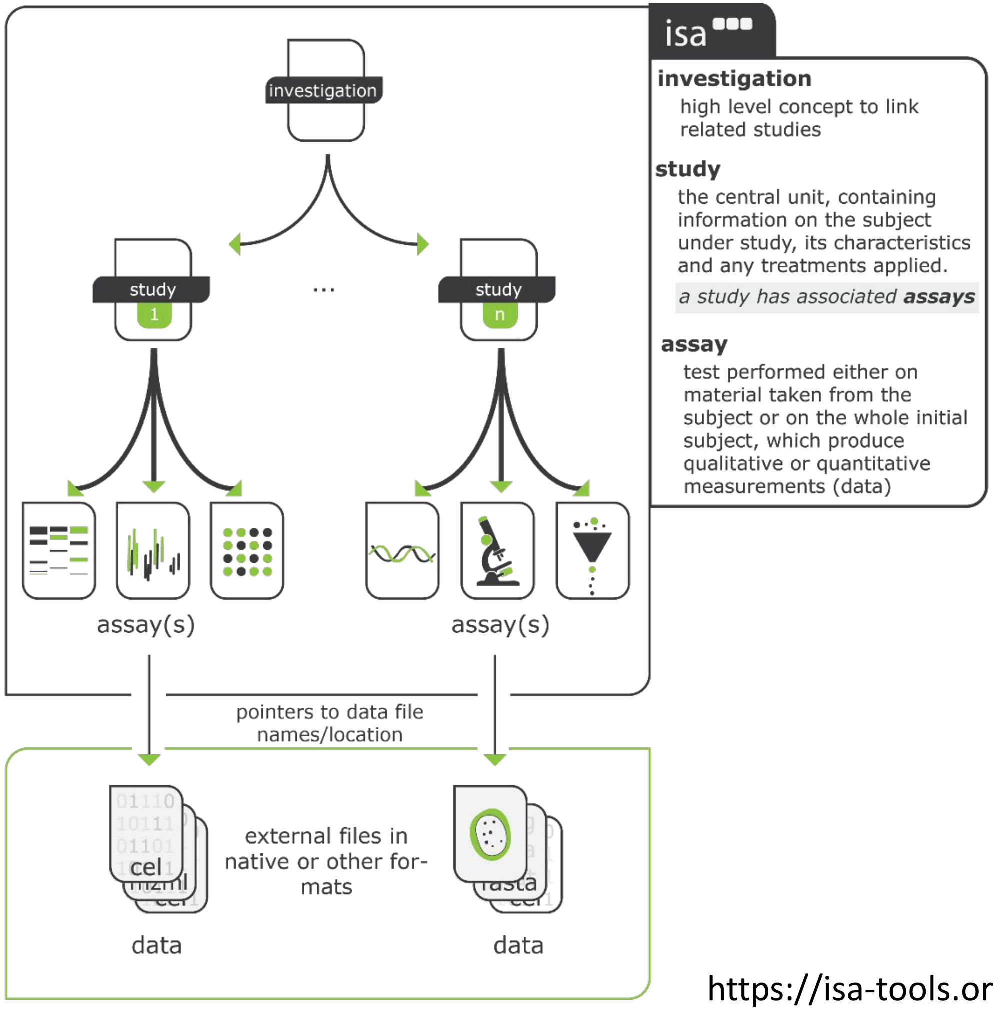
The New Medicines for Trypanosomatidic Infections - NMTrypI project aimed at obtaining new candidate drugs against Trypanosomatidic infections with appropriate efficiency from the lead phase to the final preclinical phase that are more accessible to patients.

Programme: Drug development for neglected parasitic diseases
Public web page: https://fp7-nmtrypi.eu/
Start date: 1st Feb 2014
End date: 31st Jan 2017
Organisms: Trypanosoma brucei, Trypanosoma cruzi, Leishmania donovani, Leishmania infantum, Leishmania major

Investigation - Study - Assay

isa

Specification



investigation
high level concept to link related studies

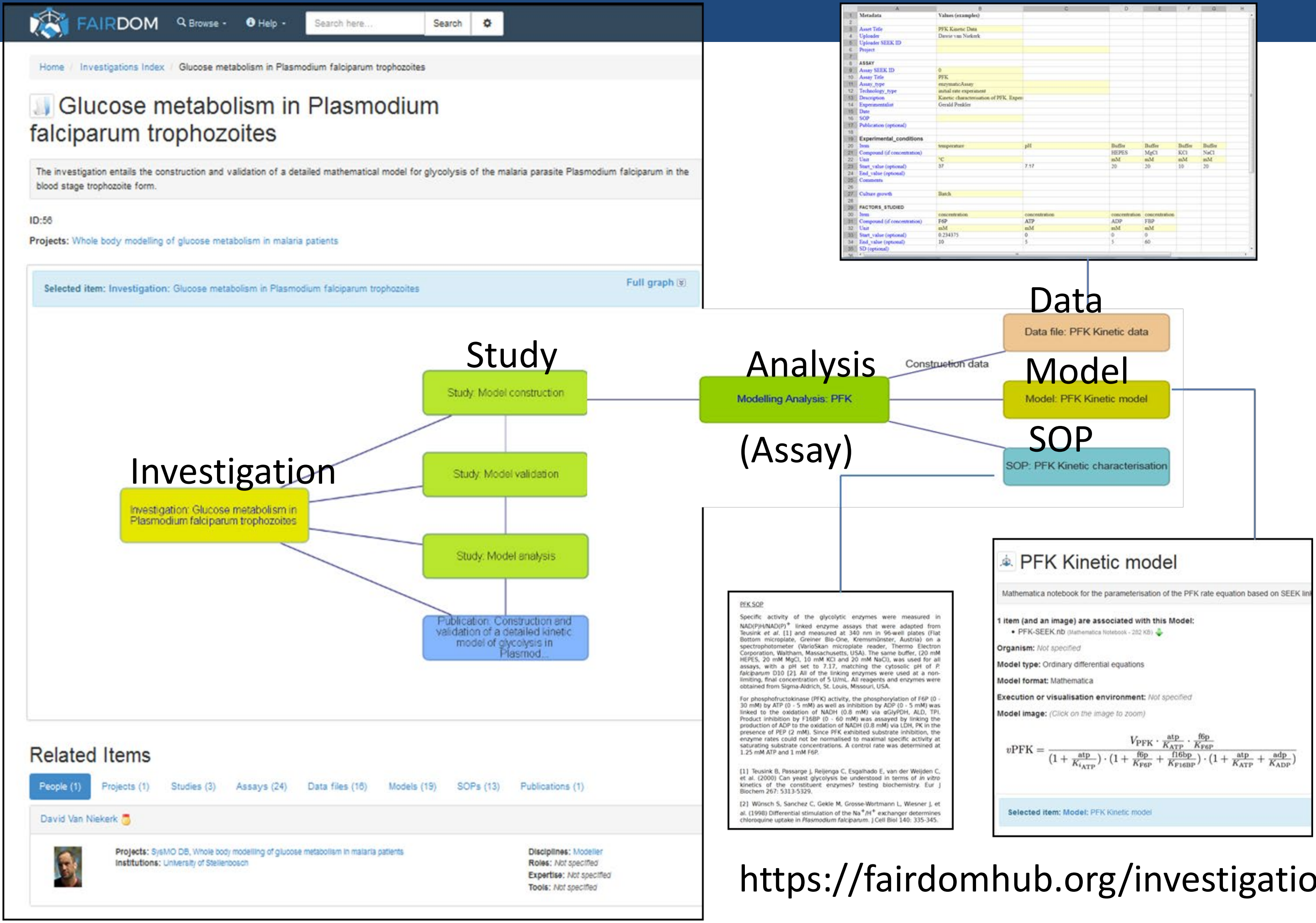
study
the central unit, containing information on the subject under study, its characteristics and any treatments applied.

*a study has associated **assays***

assay
test performed either on material taken from the subject or on the whole initial subject, which produce qualitative or quantitative measurements (data)

https://isa-tools.org/format/specification.html

Investigation - Study - Assay



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

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

	A	B	C	D	E	F	G
1	Metadata	Values (examples)					
2							
3	Asset Title	PFK Kinetic Data					
4	Uploader	Dawie van Niekerk					
5	Uploader SEEK ID						
6	Project						
7							
8	ASSAY						
9	Assay SEEK ID	0					
10	Assay Title	PFK					
11	Assay_type	enzymaticAssay					
12	Technology_type	initial rate experiment					
13	Description	Kinetic characterisation of PFK. Exper					
14	Experimentalist	Gerald Penkler					
15	Date						
16	SOP						
17	Publication (optional)						
18							
19	Experimental_conditions						
20	Item	temperature	pH	Buffer	Buffer	Buffer	Buffer
21	Compound (if concentration)			HEPES	MgCl	KCl	NaCl
22	Unit	°C		mM	mM	mM	mM
23	Start_value (optional)	37	7.17	20	20	10	20
24	End_value (optional)						
25	Comments						
26							
27	Culture growth	Batch					
28							
29	FACTORS_STUDIED						
30	Item	concentration	concentration	concentration	concentration		
31	Compound (if concentration)	F6P	ATP	ADP	FBP		
32	Unit	mM	mM	mM	mM		
33	Start_value (optional)	0.234375	0	0	0		
34	End_value (optional)	10	5	5	60		
35	SD (optional)						

PFK SOP

Specific activity of the glycolytic enzymes were measured in NAD(P)H/NAD(P)$^+$ linked enzyme assays that were adapted from Teusink *et al.* [1] and measured at 340 nm in 96-well plates (Flat Bottom microplate, Greiner Bio-One, Kremsmünster, Austria) on a spectrophotometer (VarioSkan microplate reader, Thermo Electron Corporation, Waltham, Massachusetts, USA). The same buffer, (20 mM HEPES, 20 mM MgCl, 10 mM KCl and 20 mM NaCl), was used for all assays, with a pH set to 7.17, matching the cytosolic pH of *P. falciparum* D10 [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 phosphofructokinase (PFK) activity, the phosphorylation of F6P (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 αGlyPDH, ALD, TPI. Product inhibition by F16BP (0 - 60 mM) was assayed by linking the production of ADP to the oxidation of NADH (0.8 mM) via LDH, PK in the presence of PEP (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 F6P.

[1] Teusink B, Passarge J, Reijenga C, Esgalhado E, van der Weijden C, et al. (2000) Can yeast glycolysis be understood in terms of *in vitro* kinetics of the constituent enzymes? testing biochemistry. Eur J Biochem 267: 5313-5329.

[2] Wünsch S, Sanchez C, Gekle M, Grosse-Wortmann L, Wiesner J, et al. (1998) Differential stimulation of the Na$^+$/H$^+$ exchanger determines chloroquine 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 lin

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

- PFK-SEEK.nb (Mathematica Notebook - 282 KB)

Organism: *Not specified*

Model type: Ordinary differential equations

Model format: Mathematica

Execution or visualisation environment: *Not specified*

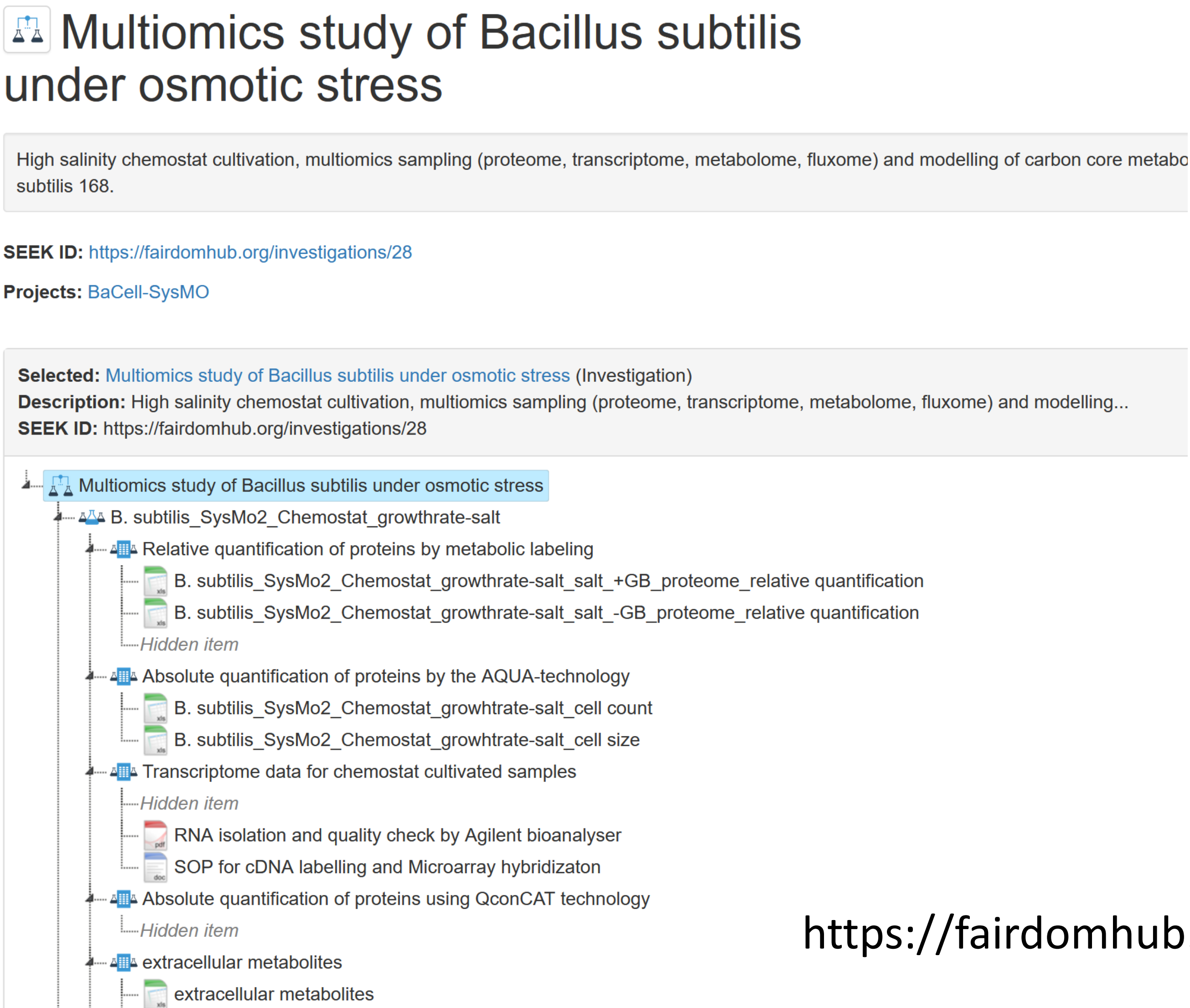
Model image: *(Click on the image to zoom)*

$$vPFK = \frac{V_{PFK}\cdot\frac{atp}{K_{ATP}}\cdot\frac{f6p}{K_{F6P}}}{\left(1+\frac{atp}{K_{i_{ATP}}}\right)\cdot\left(1+\frac{f6p}{K_{F6P}}+\frac{f16bp}{K_{F16BP}}\right)\cdot\left(1+\frac{atp}{K_{ATP}}+\frac{adp}{K_{ADP}}\right)}$$

Selected item: Model: PFK Kinetic model

https://fairdomhub.org/investigations/56

Investigation - Study - Assay



Multiomics study of Bacillus subtilis under osmotic stress

High salinity chemostat cultivation, multiomics sampling (proteome, transcriptome, metabolome, fluxome) and modelling of carbon core metabo
subtilis 168.

SEEK ID: https://fairdomhub.org/investigations/28

Projects: BaCell-SysMO

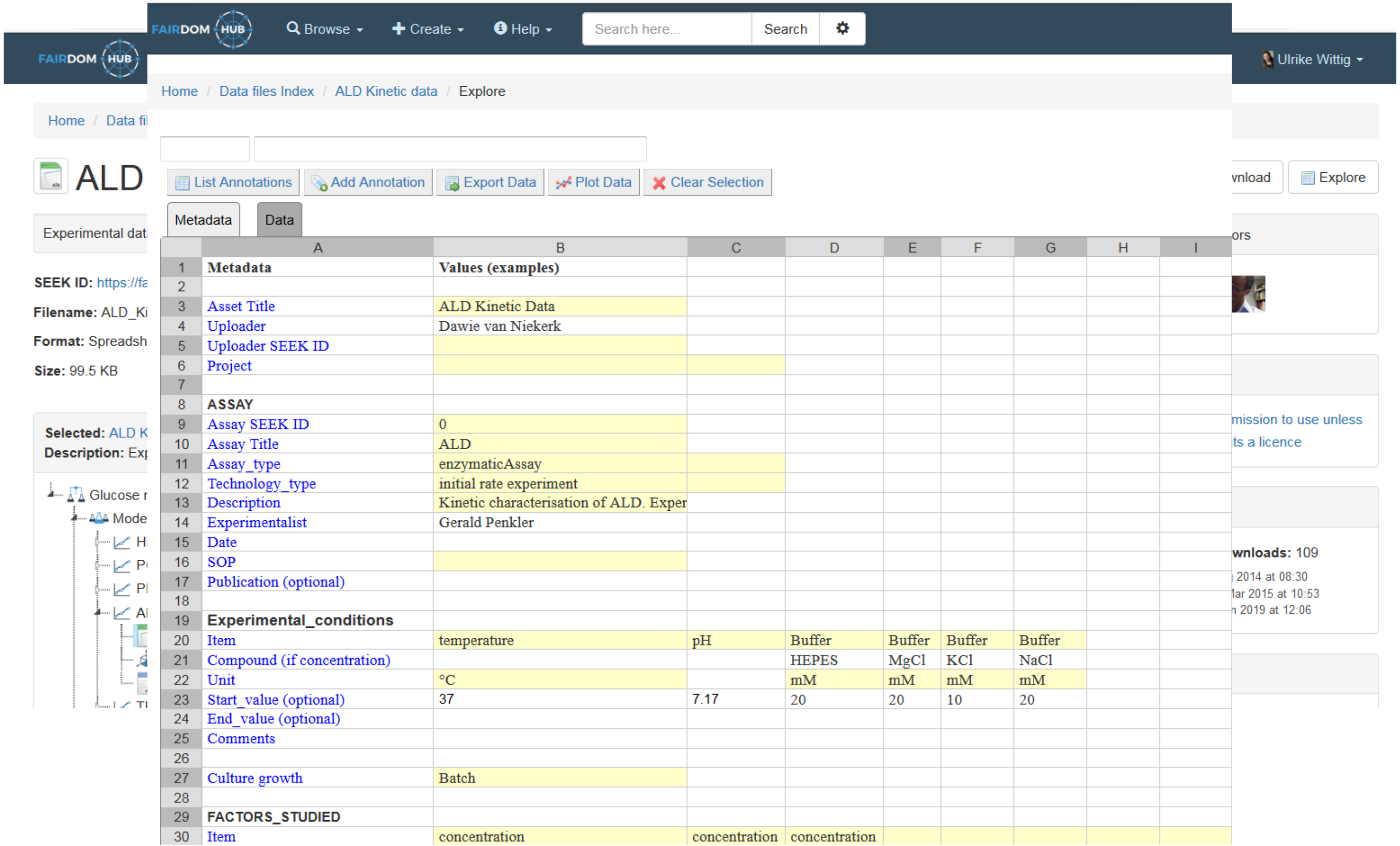
Selected: Multiomics study of Bacillus subtilis under osmotic stress (Investigation)
Description: High salinity chemostat cultivation, multiomics sampling (proteome, transcriptome, metabolome, fluxome) and modelling...
SEEK ID: https://fairdomhub.org/investigations/28

- Multiomics study of Bacillus subtilis under osmotic stress
  - B. subtilis_SysMo2_Chemostat_growthrate-salt
    - Relative quantification of proteins by metabolic labeling
      - B. subtilis_SysMo2_Chemostat_growthrate-salt_salt_+GB_proteome_relative quantification
      - B. subtilis_SysMo2_Chemostat_growthrate-salt_salt_-GB_proteome_relative quantification
      - *Hidden item*
    - Absolute quantification of proteins by the AQUA-technology
      - B. subtilis_SysMo2_Chemostat_growhtrate-salt_cell count
      - B. subtilis_SysMo2_Chemostat_growhtrate-salt_cell size
    - Transcriptome data for chemostat cultivated samples
      - *Hidden item*
      - RNA isolation and quality check by Agilent bioanalyser
      - SOP for cDNA labelling and Microarray hybridizaton
    - Absolute quantification of proteins using QconCAT technology
      - *Hidden item*
    - extracellular metabolites
      - extracellular metabolites

https://fairdomhub.org/investigations/28

Data Files, SOPs, Documents

- no file format restrictions
- some formats allow to view the content in SEEK: e.g.Excel, Word, PDF, XML, PNG



Home / Data files Index / ALD Kinetic data / Explore

Home / Data fi

ALD

Experimental dat

SEEK ID: https://fa

Filename: ALD_Ki

Format: Spreadsh

Size: 99.5 KB

Selected: ALD K
Description: Exp

Glucose r
Mode

wnloads: 109
2014 at 08:30
lar 2015 at 10:53
n 2019 at 12:06

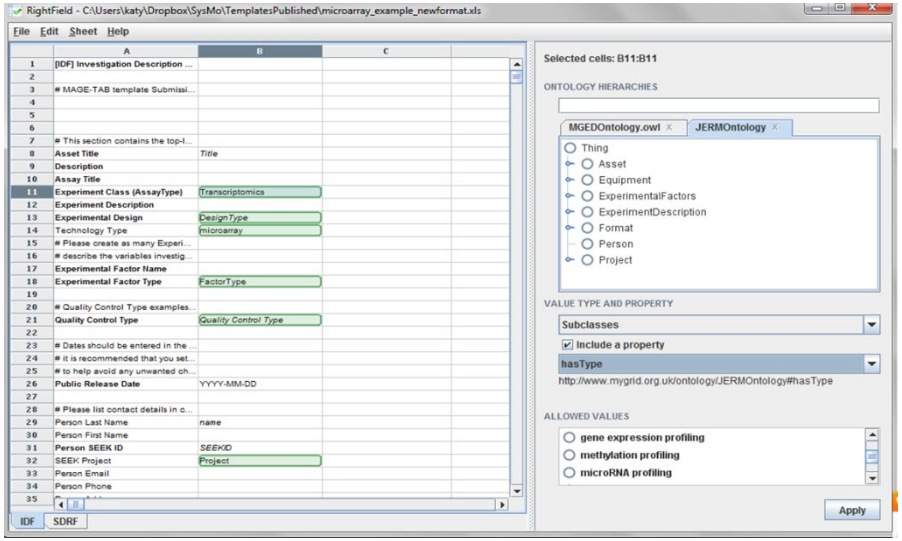
mission to use unless
ts a licence

	A	B	C	D	E	F	G	H	I
1	**Metadata**	**Values (examples)**							
2									
3	Asset Title	ALD Kinetic Data							
4	Uploader	Dawie van Niekerk							
5	Uploader SEEK ID								
6	Project								
7									
8	ASSAY								
9	Assay SEEK ID	0							
10	Assay Title	ALD							
11	Assay_type	enzymaticAssay							
12	Technology_type	initial rate experiment							
13	Description	Kinetic characterisation of ALD. Exper							
14	Experimentalist	Gerald Penkler							
15	Date								
16	SOP								
17	Publication (optional)								
18									
19	Experimental_conditions								
20	Item	temperature	pH	Buffer	Buffer	Buffer	Buffer		
21	Compound (if concentration)			HEPES	MgCl	KCl	NaCl		
22	Unit	°C		mM	mM	mM	mM		
23	Start_value (optional)	37	7.17	20	20	10	20		
24	End_value (optional)								
25	Comments								
26									
27	Culture growth	Batch							
28									
29	FACTORS_STUDIED								
30	Item	concentration	concentration	concentration					

Spreadsheet Templates

RightField

Excel enriched with ontology annotations



RightField - C:\Users\katy\Dropbox\SysMo\TemplatesPublished\microarray_example_newformat.xls

	A	B	C
1	[IDF] Investigation Description ...		
2			
3	# MAGE-TAB template Submissi...		
4			
5			
6			
7	# This section contains the top-l...		
8	**Asset Title**	*Title*	
9	**Description**		
10	**Assay Title**		
11	**Experiment Class (AssayType)**	Transcriptomics	
12	**Experiment Description**		
13	**Experimental Design**	*DesignType*	
14	Technology Type	microarray	
15	# Please create as many Experi...		
16	# describe the variables investig...		
17	**Experimental Factor Name**		
18	**Experimental Factor Type**	FactorType	
19			
20	# Quality Control Type examples...		
21	**Quality Control Type**	*Quality Control Type*	
22			
23	# Dates should be entered in the ...		
24	# it is recommended that you set...		
25	# to help avoid any unwanted ch...		
26	**Public Release Date**	YYYY-MM-DD	
27			
28	# Please list contact details in c...		
29	Person Last Name	*name*	
30	Person First Name		
31	**Person SEEK ID**	*SEEKID*	
32	SEEK Project	Project	
33	Person Email		
34	Person Phone		
35			

Selected cells: B11:B11

ONTOLOGY HIERARCHIES

- ○ Thing
  - ○ Asset
  - ○ Equipment
  - ○ ExperimentalFactors
  - ○ ExperimentDescription
  - ○ Format
  - ○ Person
  - ○ Project

VALUE TYPE AND PROPERTY

Subclasses

☑ Include a property

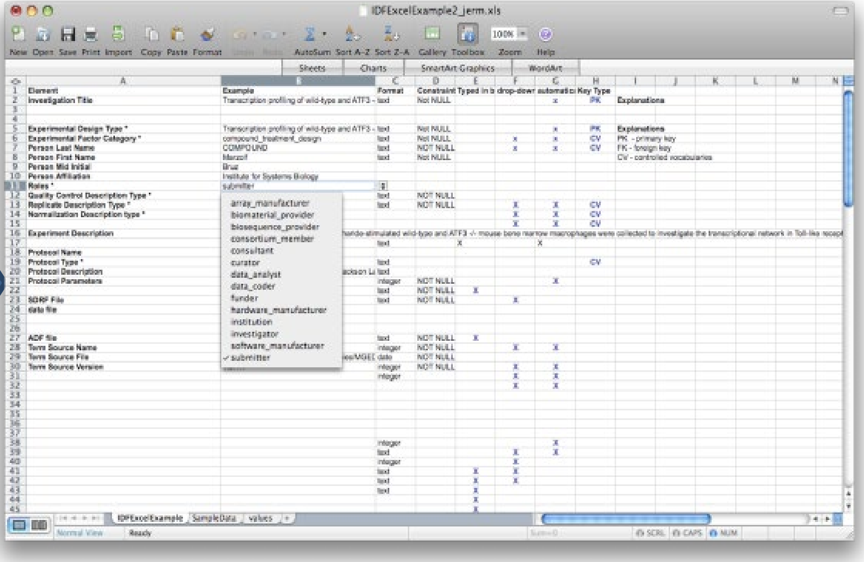
hasType

http://www.mygrid.org.uk/ontology/JERMOntology#hasType

ALLOWED VALUES

- ○ gene expression profiling
- ○ methylation profiling
- ○ microRNA profiling

Embedded ontologies in Excel templates



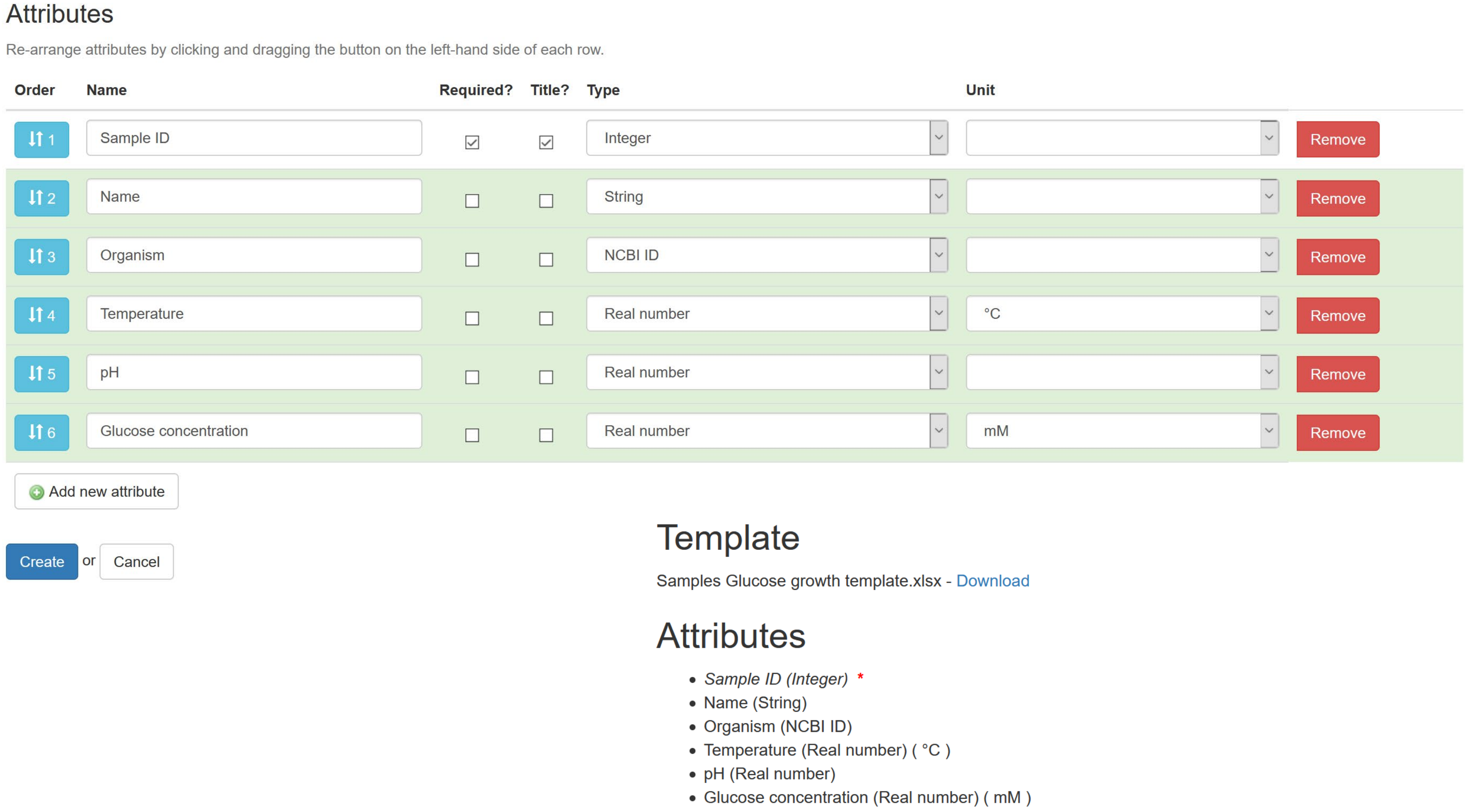
Upload, extract metadata and register

SEEK

http://www.rightfield.org.uk

Samples Types

Generation of templates for sample types



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	☑	☑	Integer		Remove
2	Name	☐	☐	String		Remove
3	Organism	☐	☐	NCBI ID		Remove
4	Temperature	☐	☐	Real number	°C	Remove
5	pH	☐	☐	Real number		Remove
6	Glucose concentration	☐	☐	Real number	mM	Remove

Template

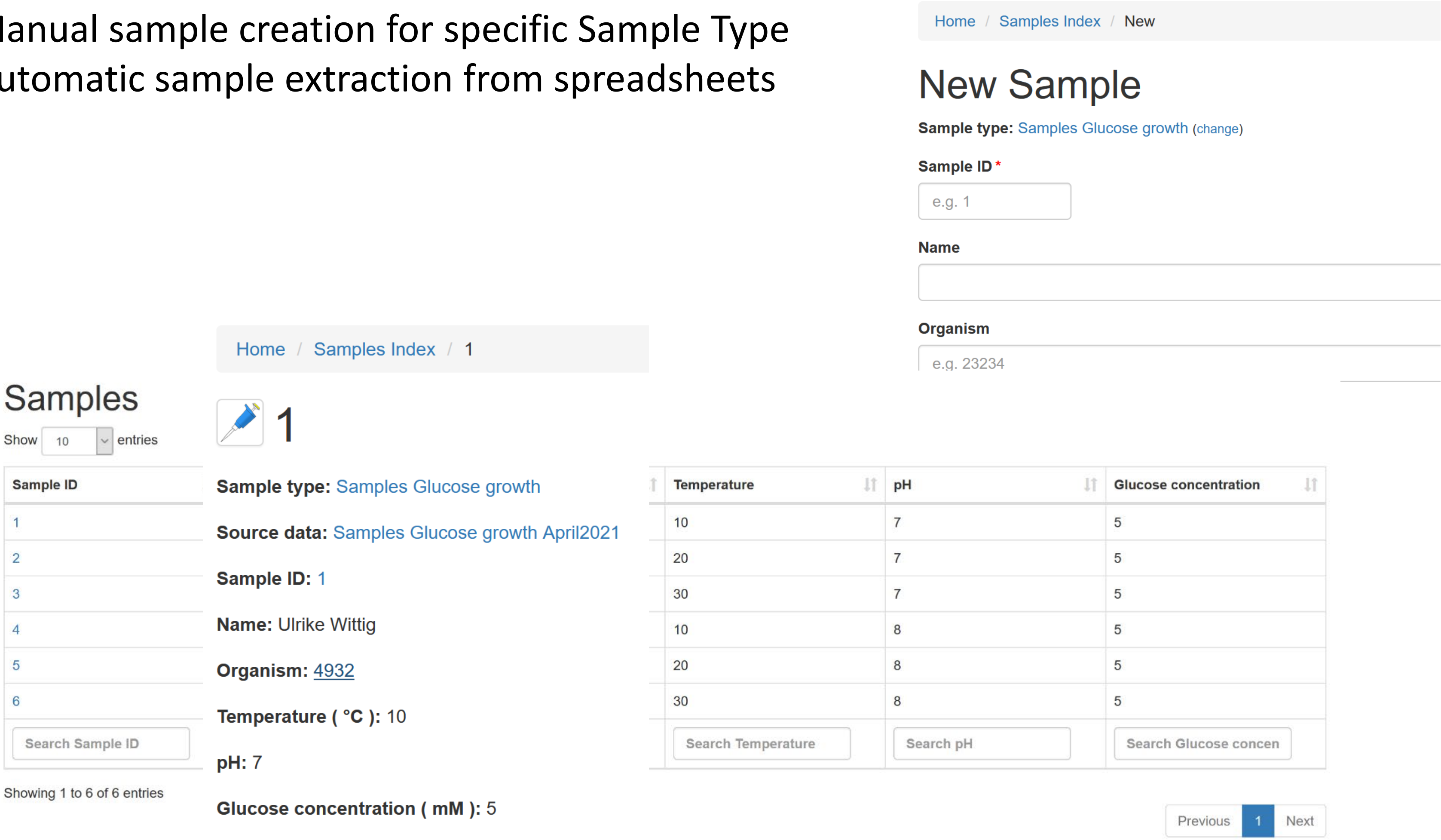
Samples Glucose growth template.xlsx - Download

Attributes

- *Sample ID (Integer)* *
- Name (String)
- Organism (NCBI ID)
- Temperature (Real number) (°C)
- pH (Real number)
- Glucose concentration (Real number) (mM)

Samples

- Manual sample creation for specific Sample Type
- Automatic sample extraction from spreadsheets



Home / Samples Index / New

New Sample

Sample type: Samples Glucose growth (change)

Sample ID *

e.g. 1

Name

Organism

e.g. 23234

Home / Samples Index / 1

1

Sample type: Samples Glucose growth

Source data: Samples Glucose growth April2021

Sample ID: 1

Name: Ulrike Wittig

Organism: 4932

Temperature (°C): 10

pH: 7

Glucose concentration (mM): 5

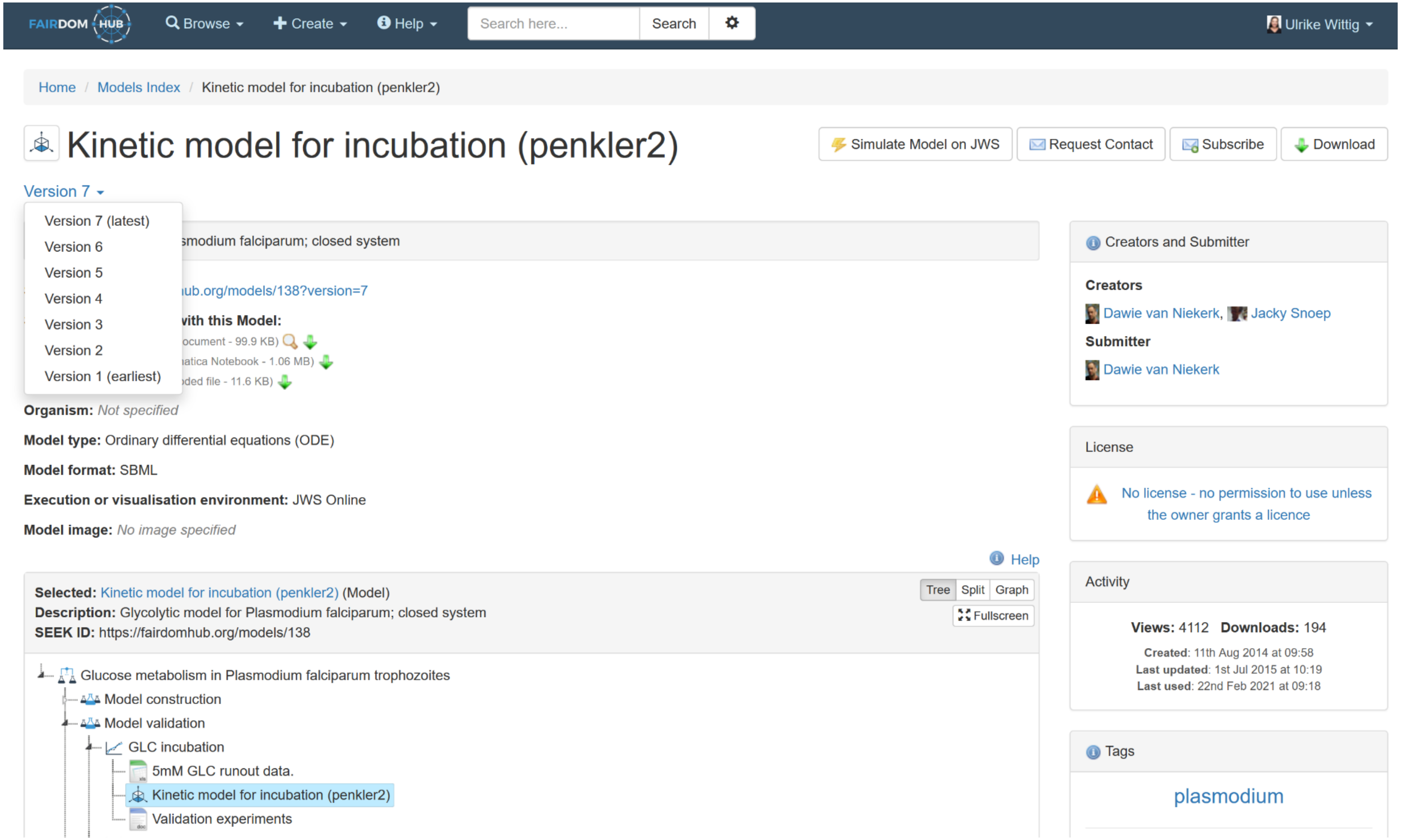
Samples

Show 10 entries

Sample ID	Temperature	pH	Glucose concentration
1	10	7	5
2	20	7	5
3	30	7	5
4	10	8	5
5	20	8	5
6	30	8	5
Search Sample ID	Search Temperature	Search pH	Search Glucose concen

Showing 1 to 6 of 6 entries

Tracking versions



Home / Models Index / Kinetic model for incubation (penkler2)

Kinetic model for incubation (penkler2)

smodium falciparum; closed system

ub.org/models/138?version=7

vith this Model:

ocument - 99.9 KB)

atica Notebook - 1.06 MB)

ded file - 11.6 KB)

Organism: *Not specified*

Model type: Ordinary differential equations (ODE)

Model format: SBML

Execution or visualisation environment: JWS Online

Model image: *No image specified*

Selected: Kinetic model for incubation (penkler2) (Model)
Description: Glycolytic model for Plasmodium falciparum; closed system
SEEK ID: https://fairdomhub.org/models/138

- Glucose metabolism in Plasmodium falciparum trophozoites
  - Model construction
  - Model validation
    - GLC incubation
      - 5mM GLC runout data.
      - Kinetic model for incubation (penkler2)
      - Validation experiments

Creators and Submitter

Creators
Dawie van Niekerk, Jacky Snoep
Submitter
Dawie van Niekerk

License

No license - no permission to use unless the owner grants a licence

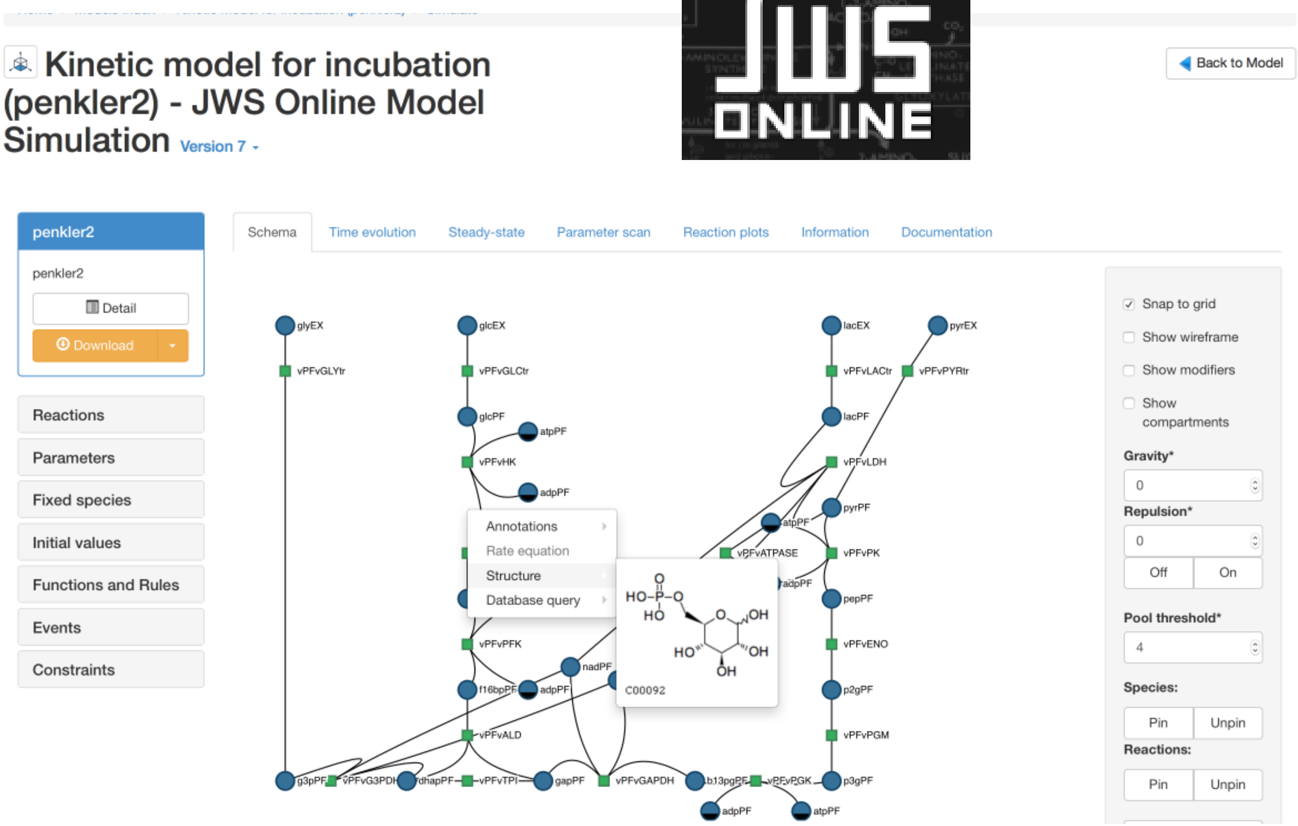
Activity

Views: 4112 **Downloads:** 194
Created: 11th Aug 2014 at 09:58
Last updated: 1st Jul 2015 at 10:19
Last used: 22nd Feb 2021 at 09:18

Tags

plasmodium

SBML Model Simulation



Kinetic model for incubation (penkler2) - JWS Online Model Simulation Version 7

Back to Model

penkler2

penkler2

Detail

Download

- Reactions
- Parameters
- Fixed species
- Initial values
- Functions and Rules
- Events
- Constraints

Schema | Time evolution | Steady-state | Parameter scan | Reaction plots | Information | Documentation

☑ Snap to grid

☐ Show wireframe

☐ Show modifiers

☐ Show compartments

Gravity* 0

Repulsion* 0

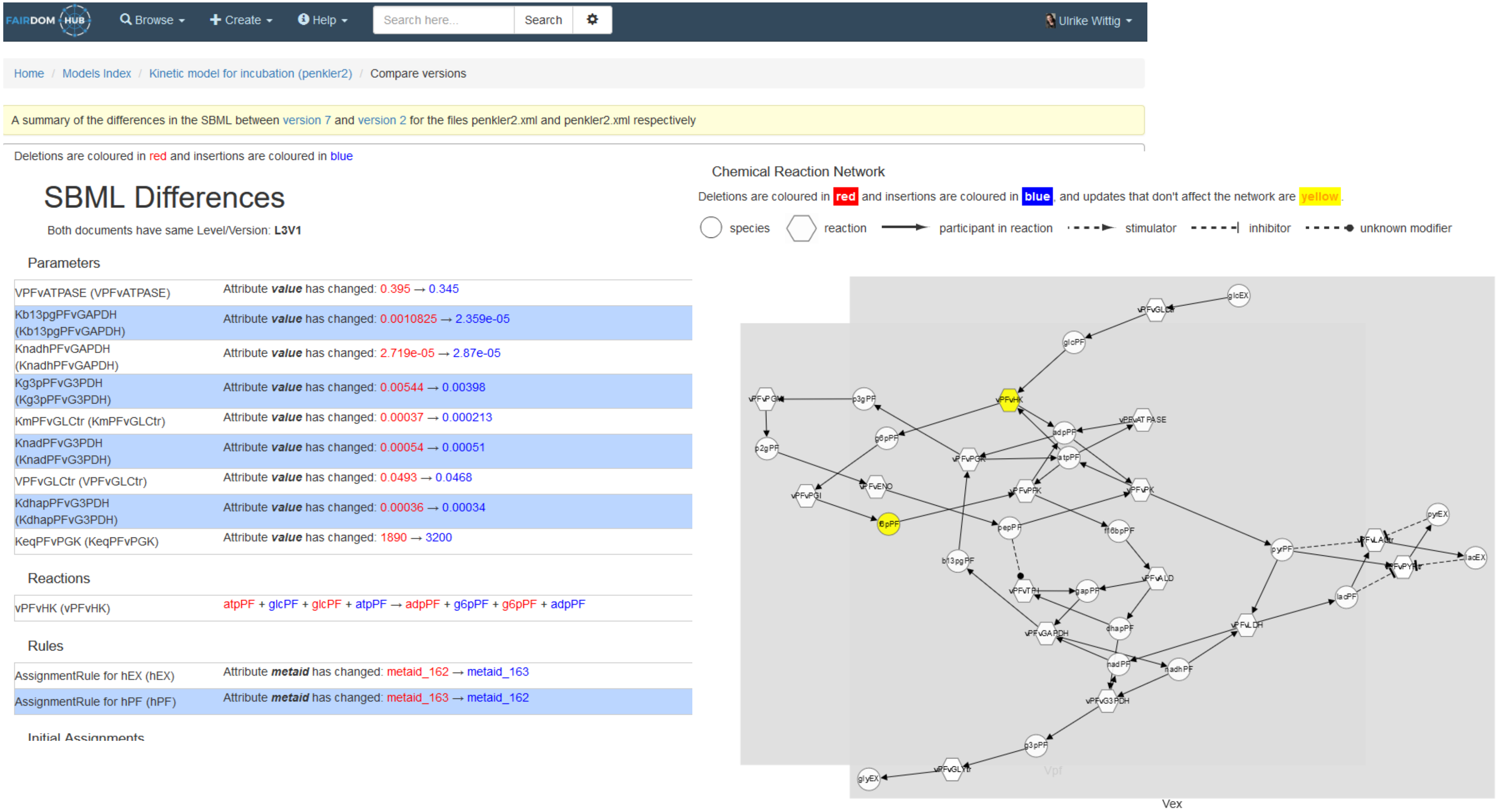
Off | On

Pool threshold* 4

Species: Pin | Unpin

Reactions: Pin | Unpin

Model comparison



A summary of the differences in the SBML between version 7 and version 2 for the files penkler2.xml and penkler2.xml respectively

Deletions are coloured in red and insertions are coloured in blue

SBML Differences

Both documents have same Level/Version: **L3V1**

Parameters

VPFvATPASE (VPFvATPASE)	Attribute ***value*** has changed: 0.395 → 0.345
Kb13pgPFvGAPDH (Kb13pgPFvGAPDH)	Attribute ***value*** has changed: 0.0010825 → 2.359e-05
KnadhPFvGAPDH (KnadhPFvGAPDH)	Attribute ***value*** has changed: 2.719e-05 → 2.87e-05
Kg3pPFvG3PDH (Kg3pPFvG3PDH)	Attribute ***value*** has changed: 0.00544 → 0.00398
KmPFvGLCtr (KmPFvGLCtr)	Attribute ***value*** has changed: 0.00037 → 0.000213
KnadPFvG3PDH (KnadPFvG3PDH)	Attribute ***value*** has changed: 0.00054 → 0.00051
VPFvGLCtr (VPFvGLCtr)	Attribute ***value*** has changed: 0.0493 → 0.0468
KdhapPFvG3PDH (KdhapPFvG3PDH)	Attribute ***value*** has changed: 0.00036 → 0.00034
KeqPFvPGK (KeqPFvPGK)	Attribute ***value*** has changed: 1890 → 3200

Reactions

vPFvHK (vPFvHK)	atpPF + glcPF + glcPF + atpPF → adpPF + g6pPF + g6pPF + adpPF

Rules

AssignmentRule for hEX (hEX)	Attribute ***metaid*** has changed: metaid_162 → metaid_163
AssignmentRule for hPF (hPF)	Attribute ***metaid*** has changed: metaid_163 → metaid_162

Initial Assignments

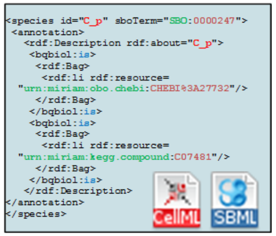
Chemical Reaction Network

Deletions are coloured in **red** and insertions are coloured in **blue**, and updates that don't affect the network are **yellow**.

○ species ⬡ reaction ⟶ participant in reaction - - -▸ stimulator - - - -| inhibitor - - - -● unknown modifier

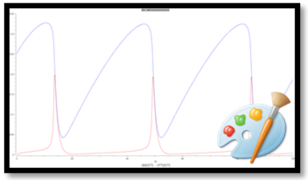
COMBINEarchive

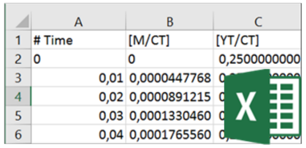
model



```
<species id="C_p" sboTerm="SBO:0000247">
 <annotation>
   <rdf:Description rdf:about="C_p">
    <bqbiol:is>
     <rdf:Bag>
      <rdf:li rdf:resource=
  "urn:miriam:obo.chebi:CHEBI%3A27732"/>
     </rdf:Bag>
    </bqbiol:is>
    <bqbiol:is>
     <rdf:Bag>
      <rdf:li rdf:resource=
  "urn:miriam:kegg.compound:C07481"/>
     </rdf:Bag>
    </bqbiol:is>
   </rdf:Description>
</annotation>
</species>
```

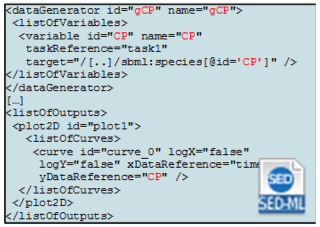
simulation results and data





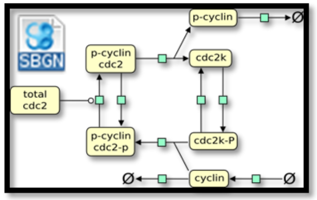
	A	B	C
1	# Time	[M/CT]	[YT/CT]
2	0	0	0,2500000000
3	0,01	0,0000447768	0
4	0,02	0,0000891215	0
5	0,03	0,0001330460	0
6	0,04	0,0001765560	0

simulation description

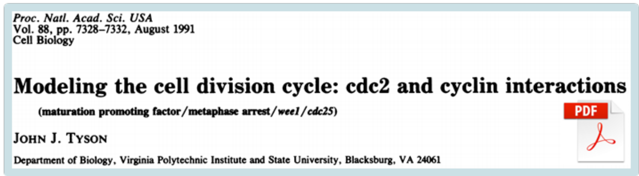


```
<dataGenerator id="gCP" name="gCP">
 <listOfVariables>
  <variable id="CP" name="CP"
   taskReference="task1"
   target="/[..]/sbml:species[@id='CP']" />
</listOfVariables>
</dataGenerator>
[…]
<listOfOutputs>
 <plot2D id="plot1">
   <listOfCurves>
    <curve id="curve_0" logX="false"
     logY="false" xDataReference="time
     yDataReference="CP" />
  </listOfCurves>
 </plot2D>
</listOfOutputs>
```

graphical representation



manuscript



Proc. Natl. Acad. Sci. USA
Vol. 88, pp. 7328–7332, August 1991
Cell Biology

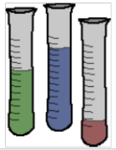
Modeling the cell division cycle: cdc2 and cyclin interactions

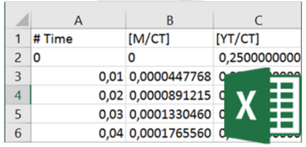
(maturation promoting factor/metaphase arrest/*wee1*/*cdc25*)

JOHN J. TYSON

Department of Biology, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061

wetlab data





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6	0,04	0,0001765560	0

BMC Bioinformatics

Software

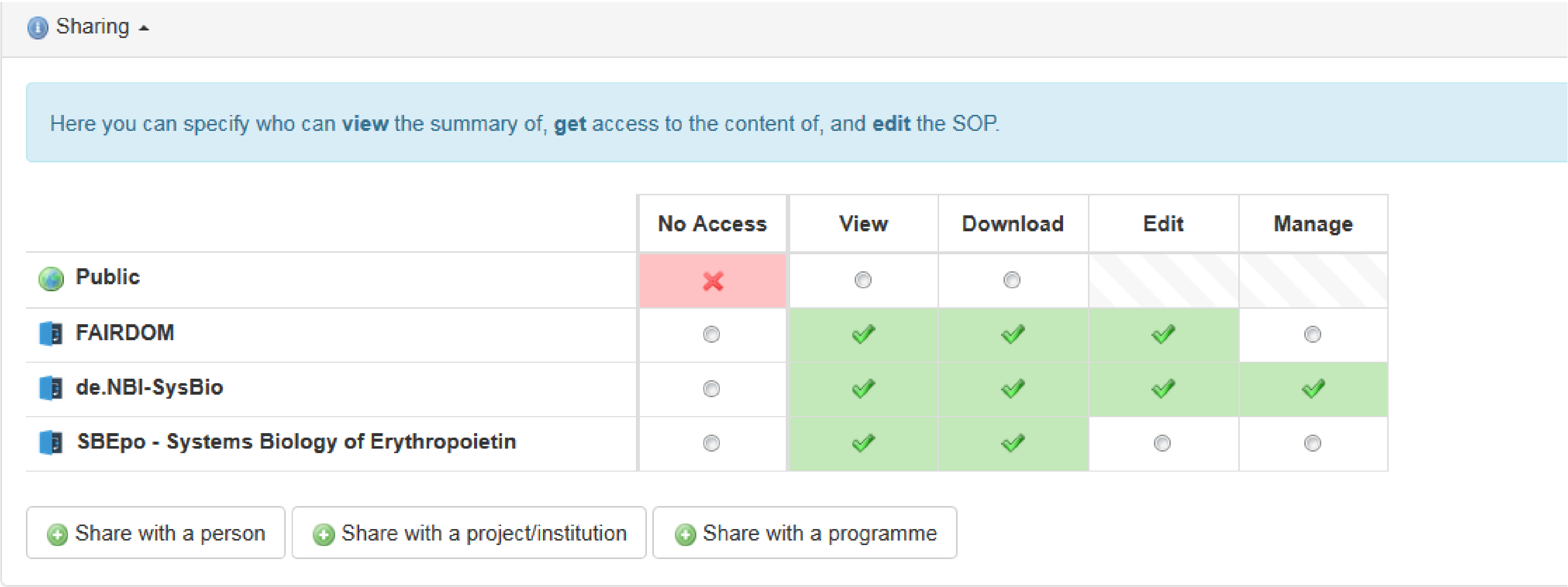
Highly accessed Open Access

COMBINE archive and OMEX format: one file to share all information to reproduce a modeling project

Frank T Bergmann[1], Richard Adams[2], Stuart Moodie[34], Jonathan Cooper[5], Mihai Glont[3], Martin Golebiewski[6], Michael Hucka[7], Camille Laibe[3], Andrew K Miller[8], David P Nickerson[8], Brett G Olivier[9], Nicolas Rodriguez[10], Herbert M Sauro[11], Martin Scharm[12], Stian Soiland-Reyes[13], Dagmar Waltemath[12], Florent Yvon[3] and Nicolas Le Novère[103]*

Bergmann, FT (2014). COMBINE archive and OMEX format: one file to share all information to reproduce a modeling project. *BMC bioinformatics*

Data Sharing



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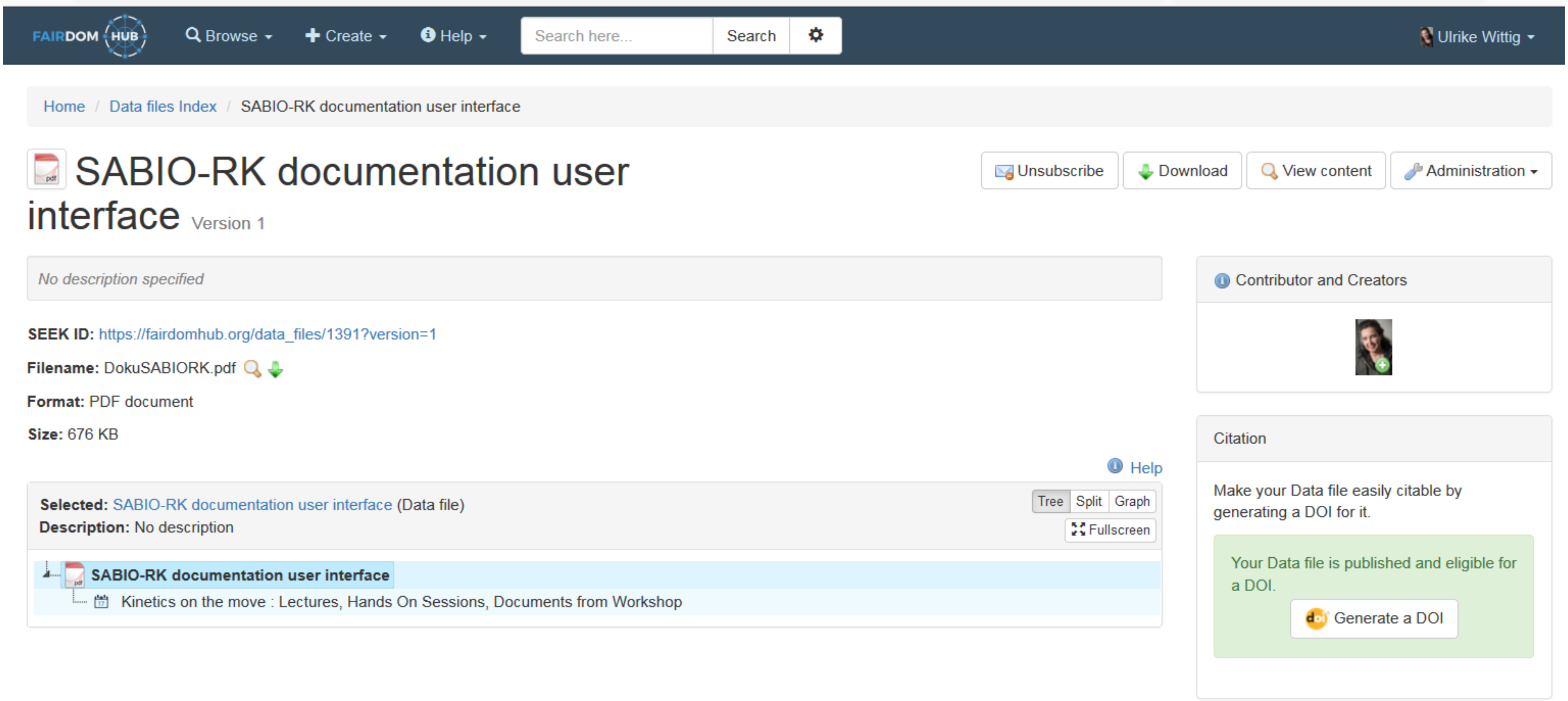
SBEpo - Systems Biology of Erythropoietin	○	✓	✓	○	○

- Keep data private
- Share within a project or programme
- Share with a institution
- Share with a person
- Share with the public

Publishing



Home / Data files Index / SABIO-RK documentation user interface

SABIO-RK documentation user interface Version 1

No description specified

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Filename: DokuSABIORK.pdf

Format: PDF document

Size: 676 KB

Selected: SABIO-RK documentation user interface (Data file)
Description: No description

SABIO-RK documentation user interface
Kinetics on the move : Lectures, Hands On Sessions, Documents from Workshop

Contributor and Creators

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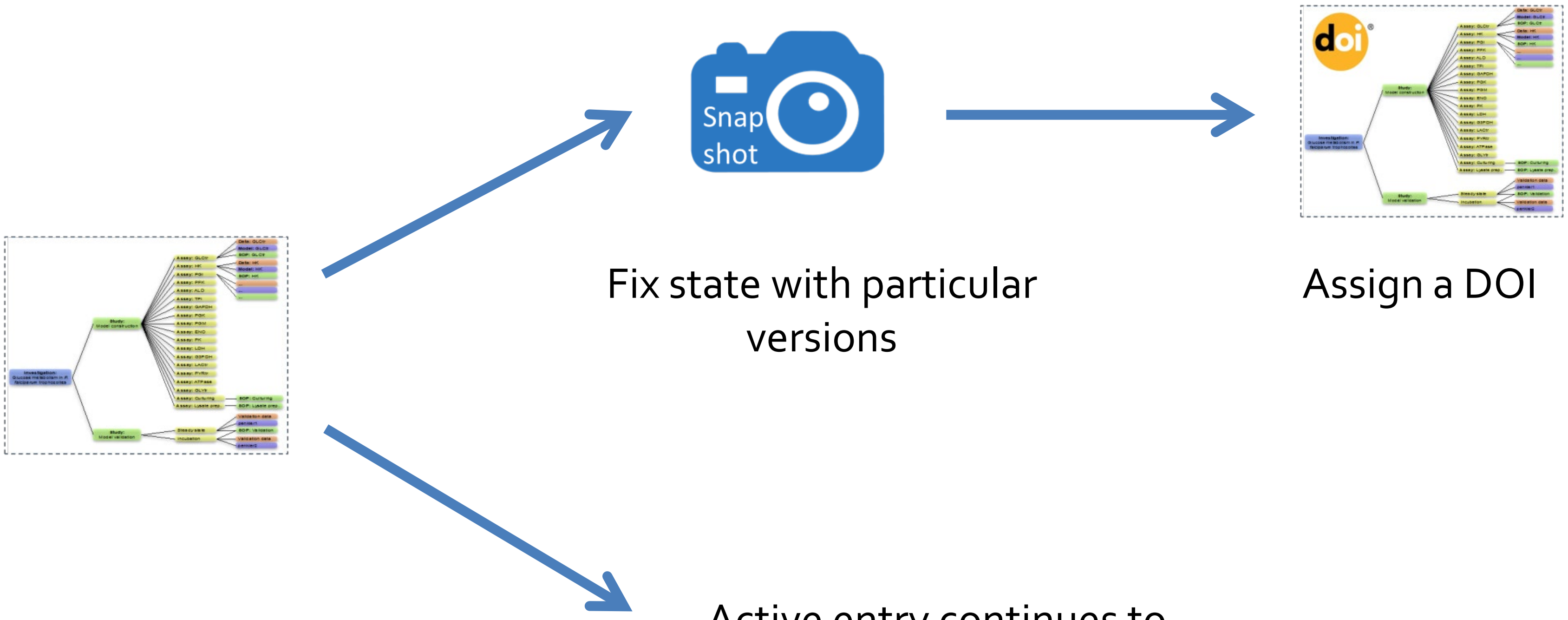

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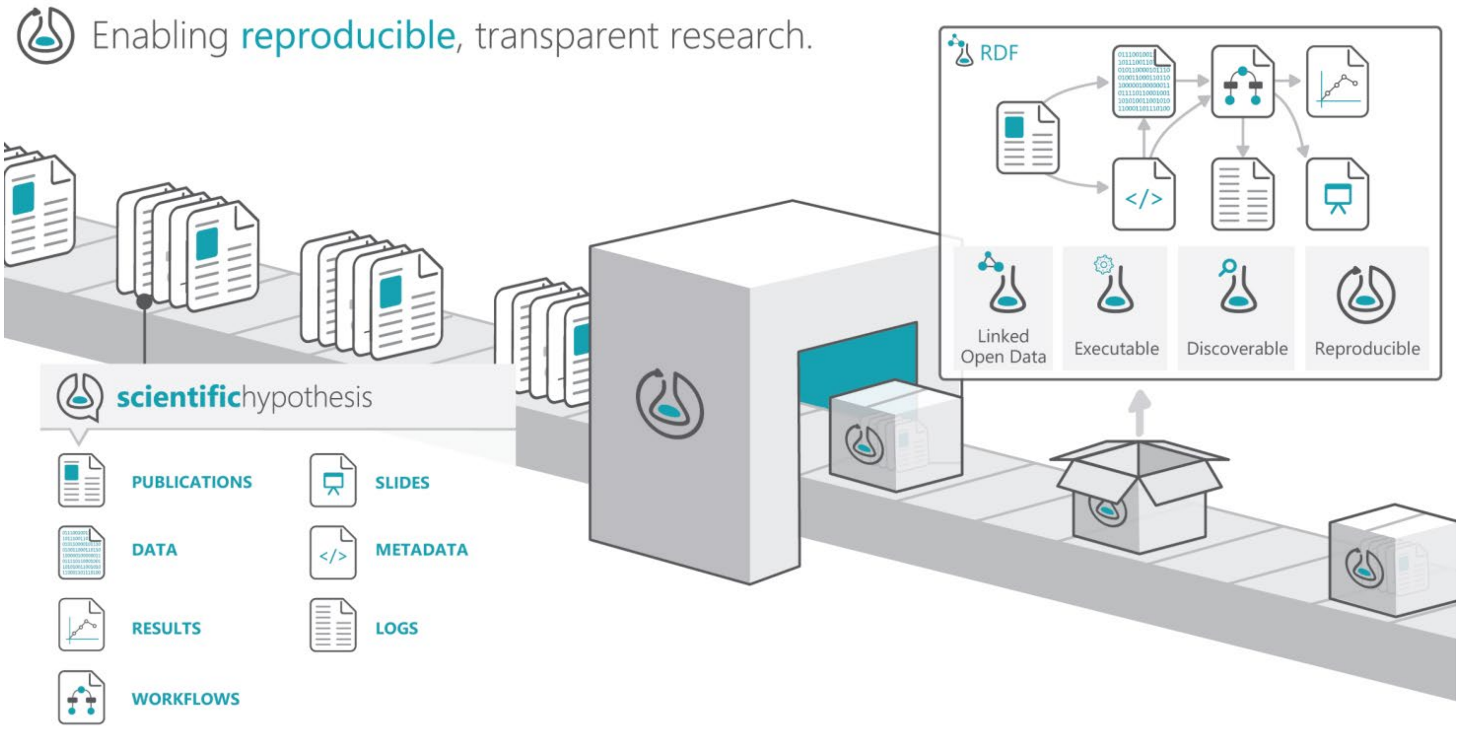

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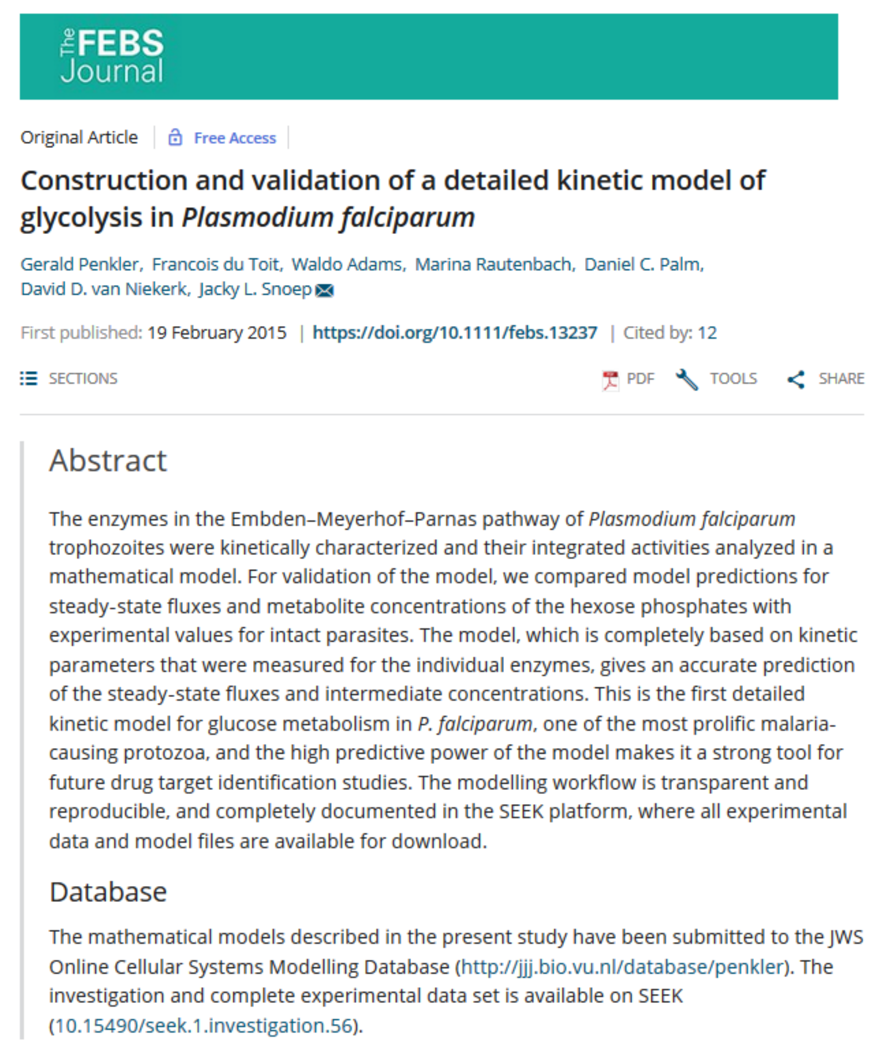


Original Article | Free Access

Construction and validation of a detailed kinetic model of glycolysis in *Plasmodium falciparum*

Gerald Penkler, Francois du Toit, Waldo Adams, Marina Rautenbach, Daniel C. Palm, David D. van Niekerk, Jacky L. Snoep

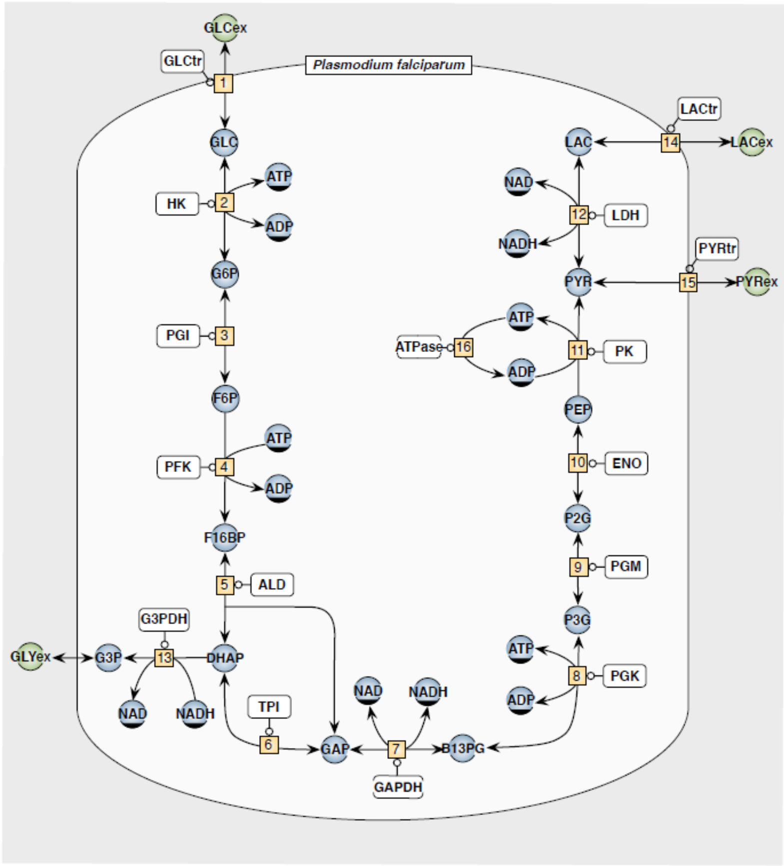
First published: 19 February 2015 | https://doi.org/10.1111/febs.13237 | Cited by: 12

Abstract

The enzymes in the Embden–Meyerhof–Parnas pathway of *Plasmodium falciparum* trophozoites were kinetically characterized and their integrated activities analyzed in a mathematical model. For validation of the model, we compared model predictions for steady-state fluxes and metabolite concentrations of the hexose phosphates with experimental values for intact parasites. The model, which is completely based on kinetic parameters that were measured for the individual enzymes, gives an accurate prediction of the steady-state fluxes and intermediate concentrations. This is the first detailed kinetic model for glucose metabolism in *P. falciparum*, one of the most prolific malaria-causing protozoa, and the high predictive power of the model makes it a strong tool for future drug target identification studies. The modelling workflow is transparent and reproducible, and completely documented in the SEEK platform, where all experimental data and model files are available for download.

Database

The mathematical models described in the present study have been submitted to the JWS Online Cellular Systems Modelling Database (http://jjj.bio.vu.nl/database/penkler). The investigation and complete experimental data set is available on SEEK (10.15490/seek.1.investigation.56).



More than simple supplementary materials

the FEBS Journal

Construction and validation of a detailed kinetic model of glycolysis in *Plasmodium falciparum*

Gerald Penkler[1,2], Francois du Toit[1], Waldo Adams[1], Marina Rautenbach[1], Daniel C. Palm[1],
David D. van Niekerk[1] and Jacky L. Snoep[1,2,3]

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3 MIB, University of Manchester, UK

Keywords
enzyme kinetics; glucose metabolism; model workflow; mathematical model; systems biology

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doi:10.1111/febs.13237

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Introduction

Despite several attempts at a complete eradication of the disease, malaria is still killing more than half a million people per year, mostly small children in sub-saharan Africa (World Health Organisation Malaria report 2013, http://www.who.int/malaria/publications/world_malaria_report_2013/en/). The disease is caused by parasitic protozoa of the *Plasmodium* genus, which have a complicated life cycle consisting of an insect vector and vertebrate host [1]. In the human host, parasite sporozoites first invade liver cells, but the malaria disease symptoms manifest only at a later stage during multiplication of the asexual stages of the parasite in red blood cells (RBCs). The blood life cycle consists of ring, trophozoite and schizont stages, and subsequent

Abbreviations

2PG, 2-phosphoglycerate; 3PG, 3-phosphoglycerate; ALD, fructose-bisphosphate aldolase; B13PG, 1,3-bisphosphoglycerate; DHAP, glycerone phosphate; ENO, phosphopyruvate hydratase; F16BP, fructose 1,6-bisphosphate; F6P, fructose 6-phosphate; G3P, glycerol 3-phosphate; G3PDH, glycerol 3-phosphate dehydrogenase; G6P, glucose 6-phosphate; GAP, D-glyceraldehyde 3-phosphate; GAPDH, glyceraldehyde 3-phosphate dehydrogenase; GLC, glucose; GLY, glycerol; HK, hexokinase; LAC, lactate; LDH, lactate dehydrogenase; MCT, monocarboxylate transporter; ODE, ordinary differential equation; PEP, phosphoenolpyruvate; PFK, 6-phosphofructokinase; PGI, glucose 6-phosphate isomerase; PGK, phosphoglycerate kinase; PGM, phosphoglycerate mutase; PK, pyruvate kinase; PYR, pyruvate; RBC, red blood cell; TCA, tricarboxylic acid; TPI, triose-phosphate isomerase.

FEBS Journal **282** (2015) 1481–1511 © 2015 FEBS 1481

Penkler, G., du Toit, F., Adams, W., Rautenbach, M., Palm, D. C., van Niekerk, D. D. and Snoep, J. L. (2015), Construction and validation of a detailed kinetic model of glycolysis in *Plasmodium falciparum*. FEBS J, 282: 1481–1511. doi:10.1111/febs.13237

16 datafiles (kinetic, flux inhibition, runout)

19 models (kinetics, validation)

13 SOPs

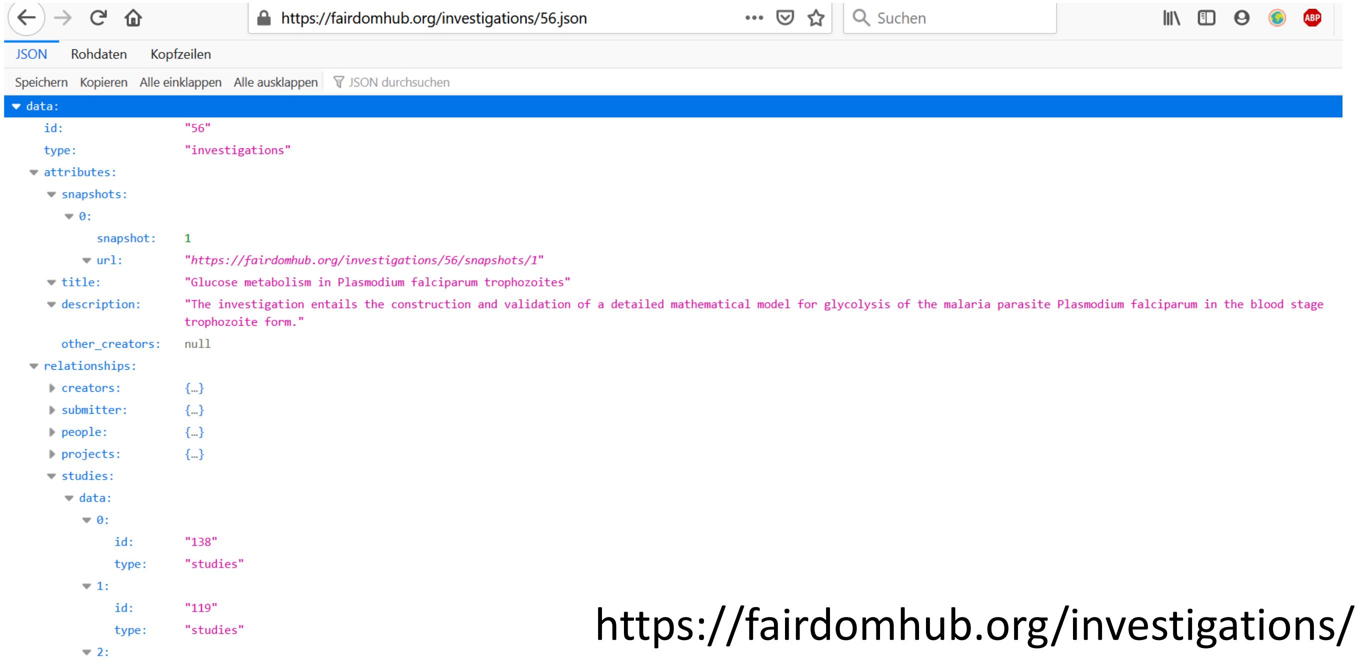
3 studies (model analysis, construction, validation)

24 assays/analyses (simulations, model characterisations)

API

JSON Application Programming Interface (API) allows programmatic access for

→ searching, listing, reading, updating, creating



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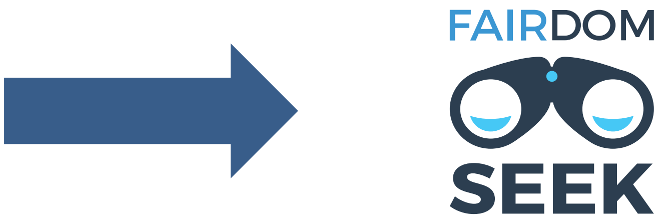
FAIRDOM-SEEK Integration

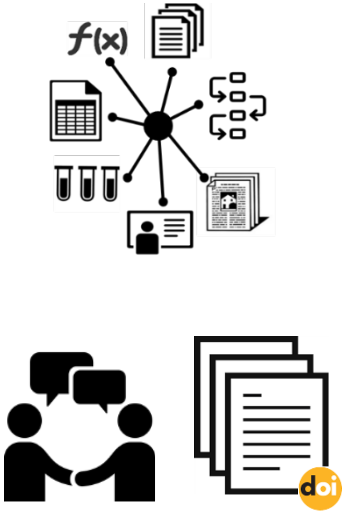
Back end

Onsite storage & analytics

Front end

FAIRDOM-SEEK



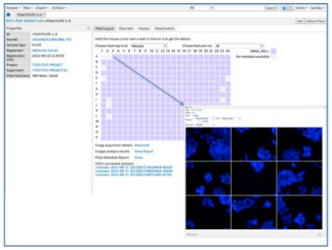


Tracking, data analytic pipelines,
Extract, Transform and Load direct from the instruments, large data management
LIMS, auto-archiving

Web-based portal
Project controlled spaces
Metadata catalogue, Yellow pages
Results repository
Sharing and publication

Back end

Instrument Data Management, LIMS, ELN



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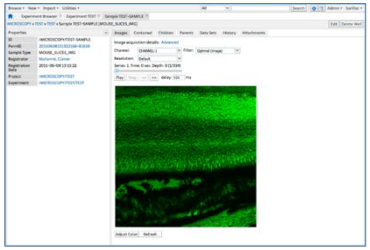

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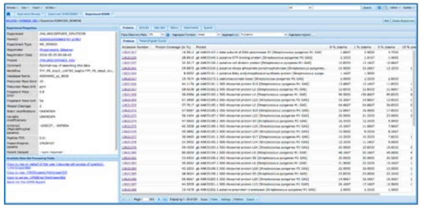
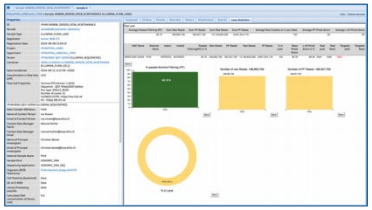


Proteomics



Sequencing

- samples
- protocols
- instruments
- data management
- experimental description

openBIS
Biology Information System

Electronic Laboratory Notebook and Laboratory Information Management System (ELN-LIMS)
https://csb.ethz.ch/tools/software/openbis-lims-eln.html

NeLS
Norwegian e-Infratructure for Life Sciences

Norway's national e-Infrastructure for Life Science
https://nels.bioinfo.no/

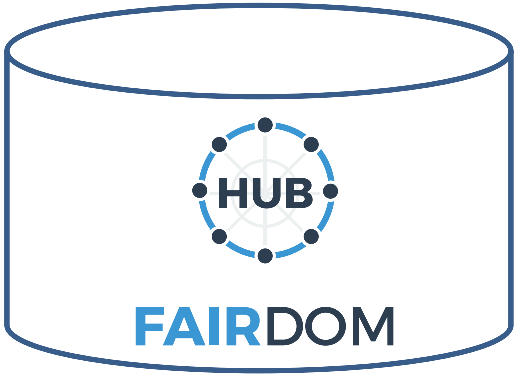
Front End

Find, Access and Organise assets

FAIRDOM
SEEK

- Upload data
- Link to data regardless of physical store
- Sharing
- ISA structure
- Yellow pages and collaboration
- Supplementary data for publications
- Standards-compliant

Project-specific local instances or central FAIRDOMHub



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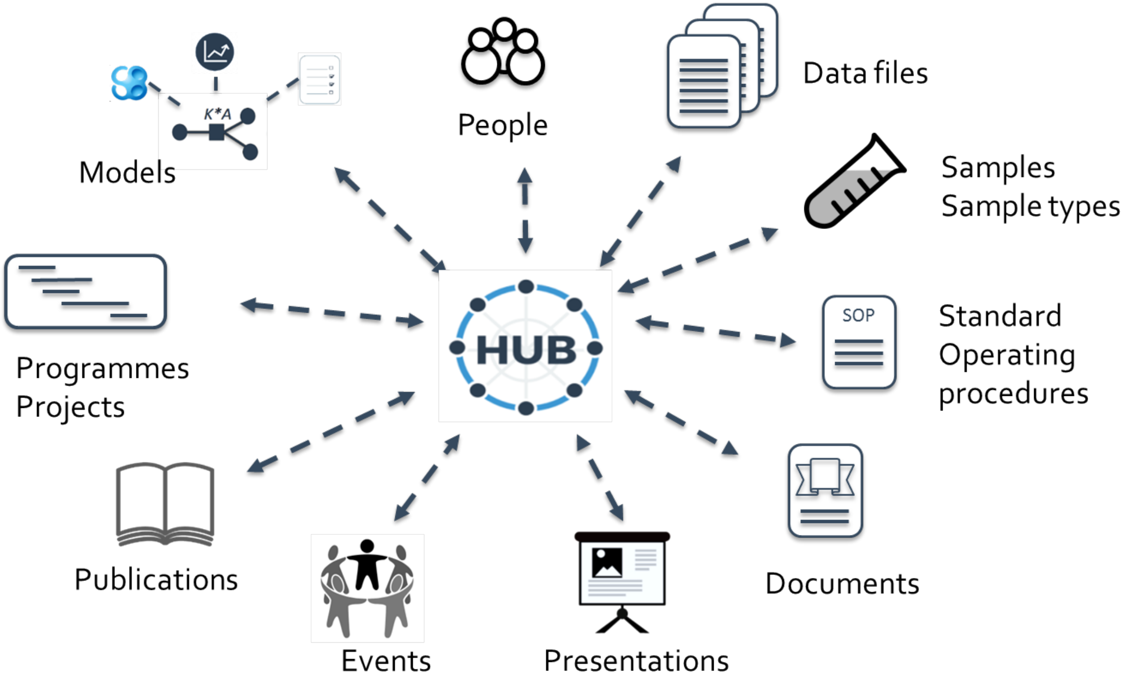
SOPs	382
Documents	774
Sample types	35
Presentations	1049
Publications	538
Events	266



https://fairdomhub.org/

Being FAIR in FAIRDOM-SEEK

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Interoperate	Rich metadata, standards compliance Consistent reporting – ISA Integration with other resources, archives, tools Export packages
Reuse	Secure sharing space Long term retention Reproducible publication

Questions?

ulrike.wittig@h-its.org

KTS

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