FAIRDOM

FAIRDOM: Promoting and Supporting FAIR Data and Model Management in Systems Biology

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HITS

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The University of Manchester

ETH Zürich

FAIRDOM

www.fair-dom.org

Share FAIR Data, Processes and Models

Findable

Accessible

Interoperable

Reusable

Data

Operating procedures

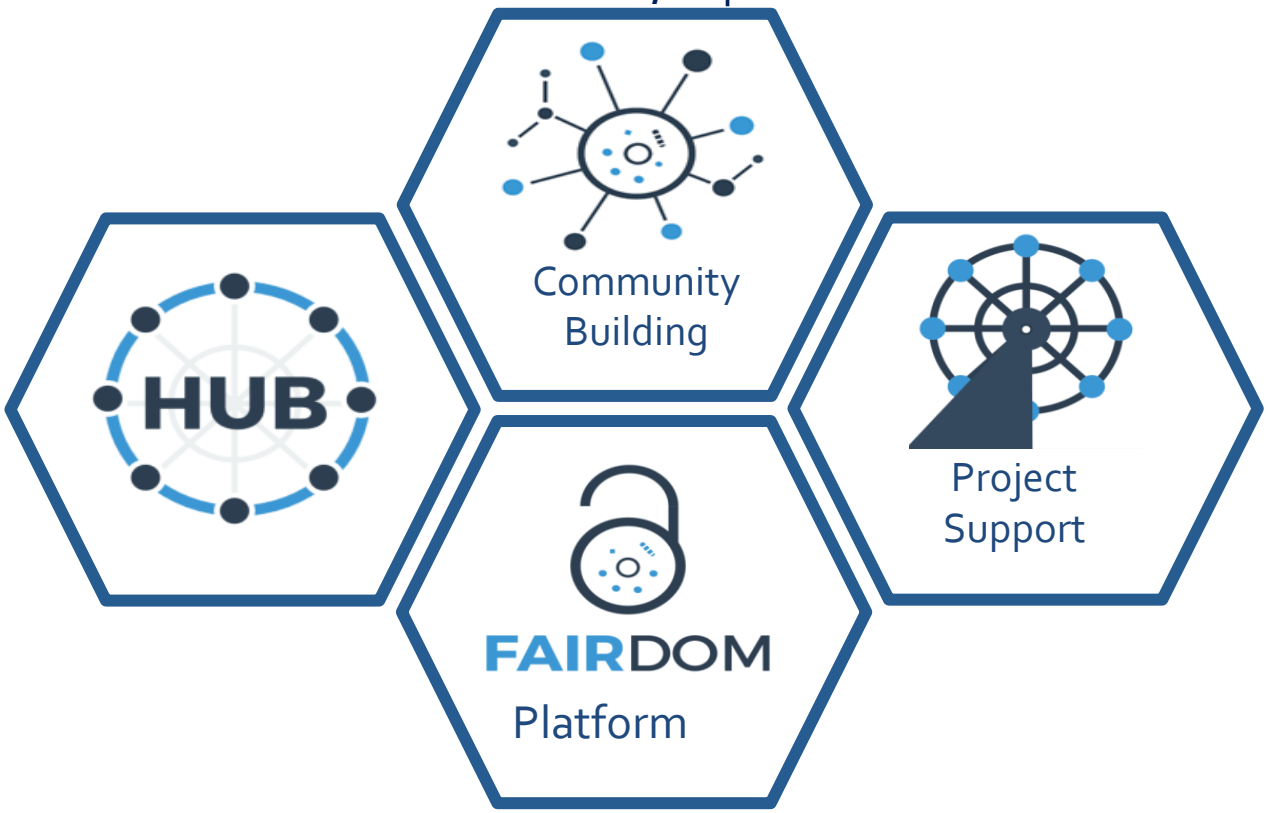
Models

HITS

FAIRDOM Summary

Skills, Capacity Building, Events
Dissemination, Exploitation

Showcase,
Sharing,
Publishing
Retention of
results
Compliance



Data
Management
Planning, and
assessment
Tailored
support,
curation,
Policies

HITS

Manage data in-house and Use Public Resources
Analysis, Tracking, Reuse, Exchange

FAIRDOM

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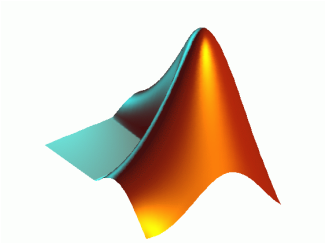
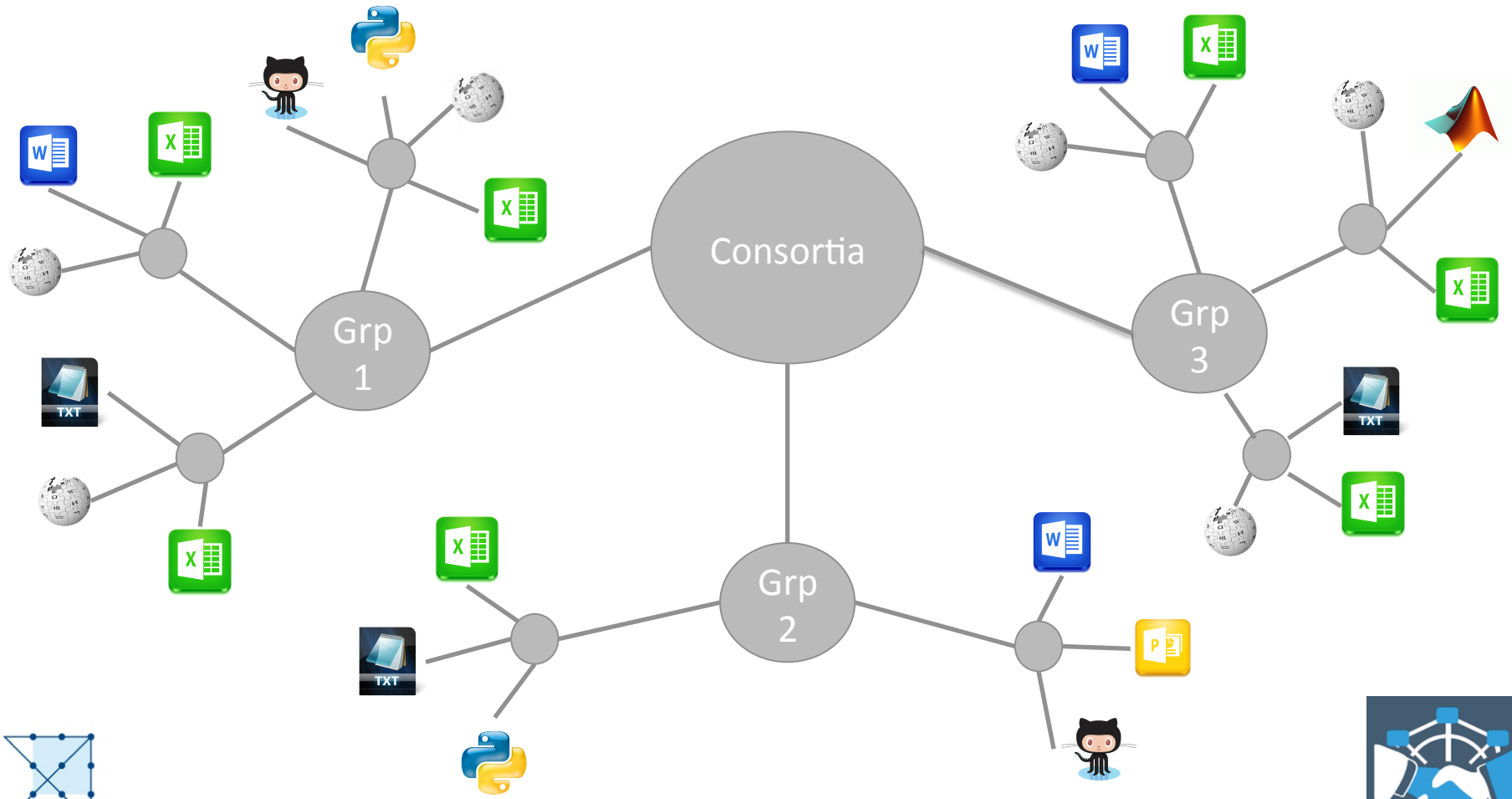
STANDARD TOOLING AND PUBLICATION SUPPORT

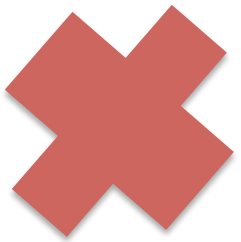
Researchers generate, record, store and share data in many formats.

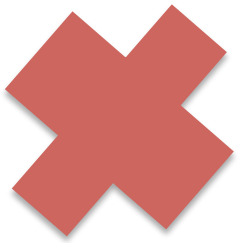


Researcher have their own preferences.



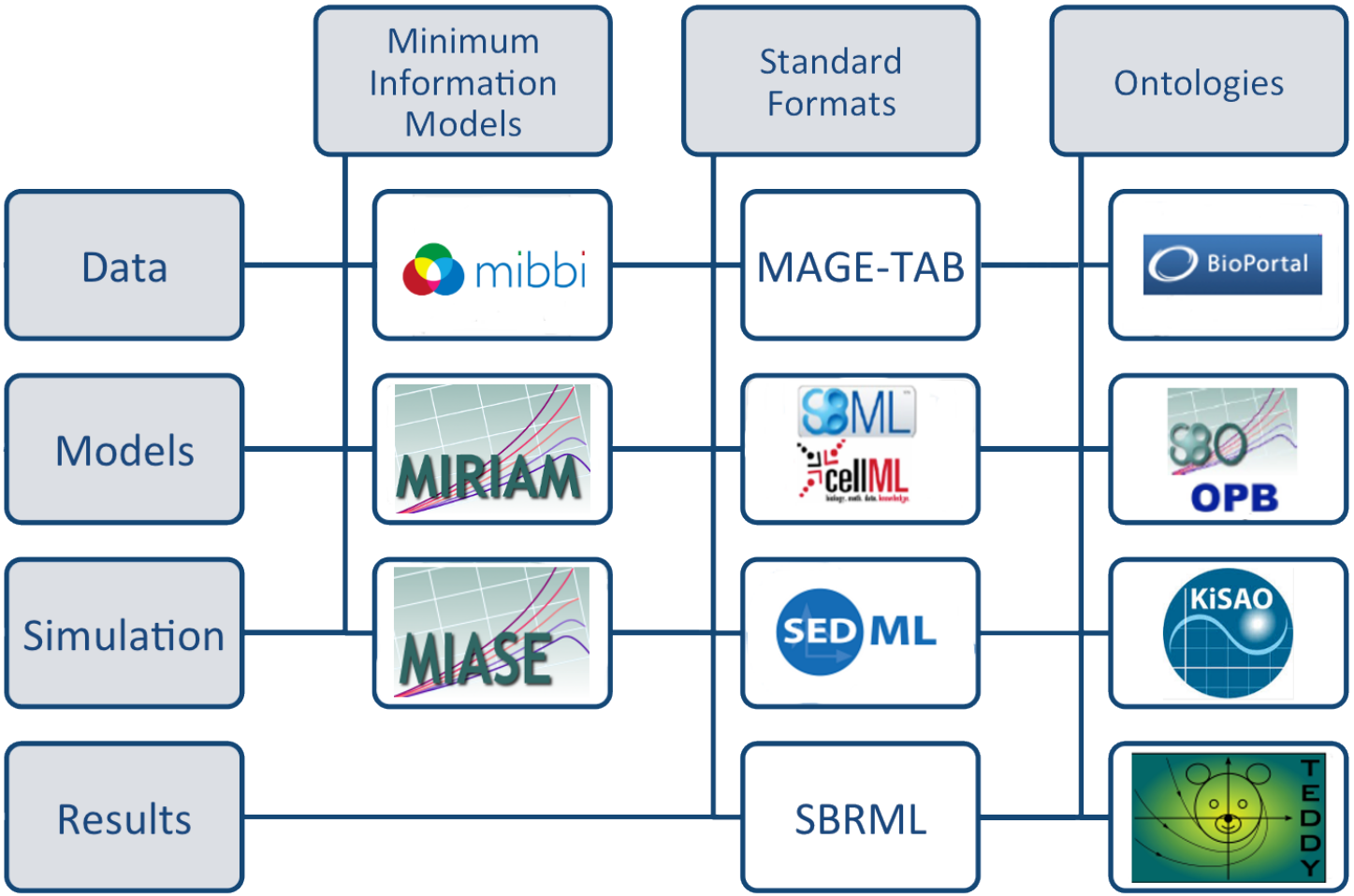
This type of data management does not adhere to FAIR principles.

INTEROPERABLE 

REUSABLE 

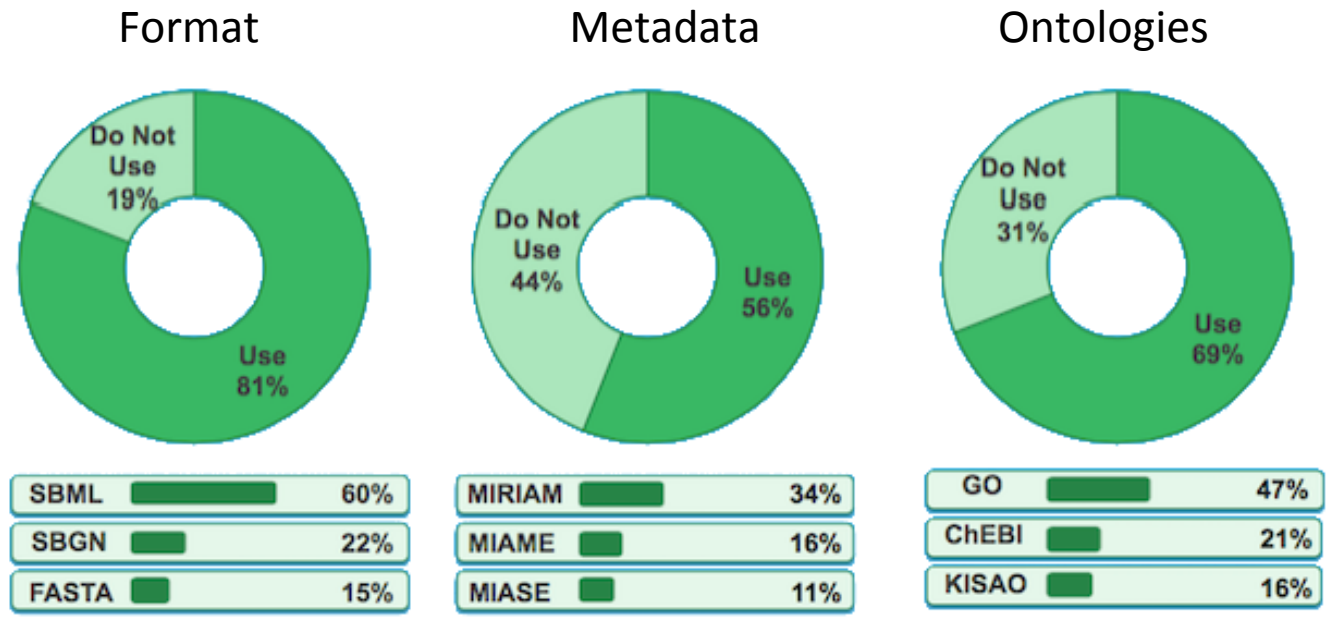
HITS

Standards are available that help to improve understanding and exchange.



Nicolas Le Novère, Babraham Institute, UK.

…but we know that researchers do not always use these.



*top three most popular

The evolution of standards and data management practices in systems biology (2015). Stanford, Wolstencroft, Golebiewski*, et al.*, Molecular Systems Biology, 11(12):851

Tooling can help to reduce the barriers to implementing standards.

COPASI

RightField

SWS ONLINE

libSBML

CellDesigner.org

cellML

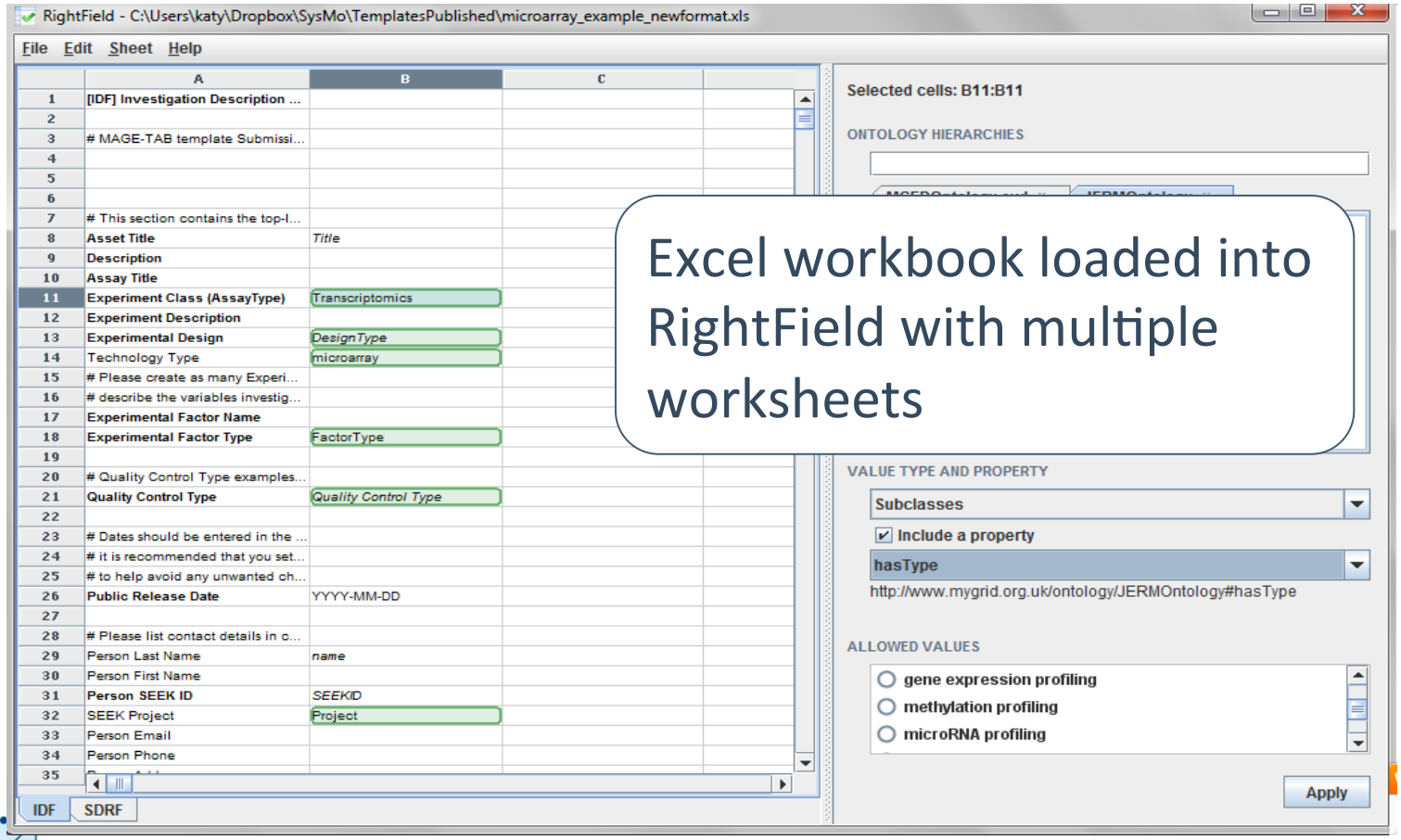
HITS

We provide Tooling for annotating spreadsheets.

RightField

HITS

We use it to generate templates for different types of assay data.



HITS

This type of data management does not adhere to FAIR principles.

INTEROPERABLE ✔

REUSABLE ✔

HITS

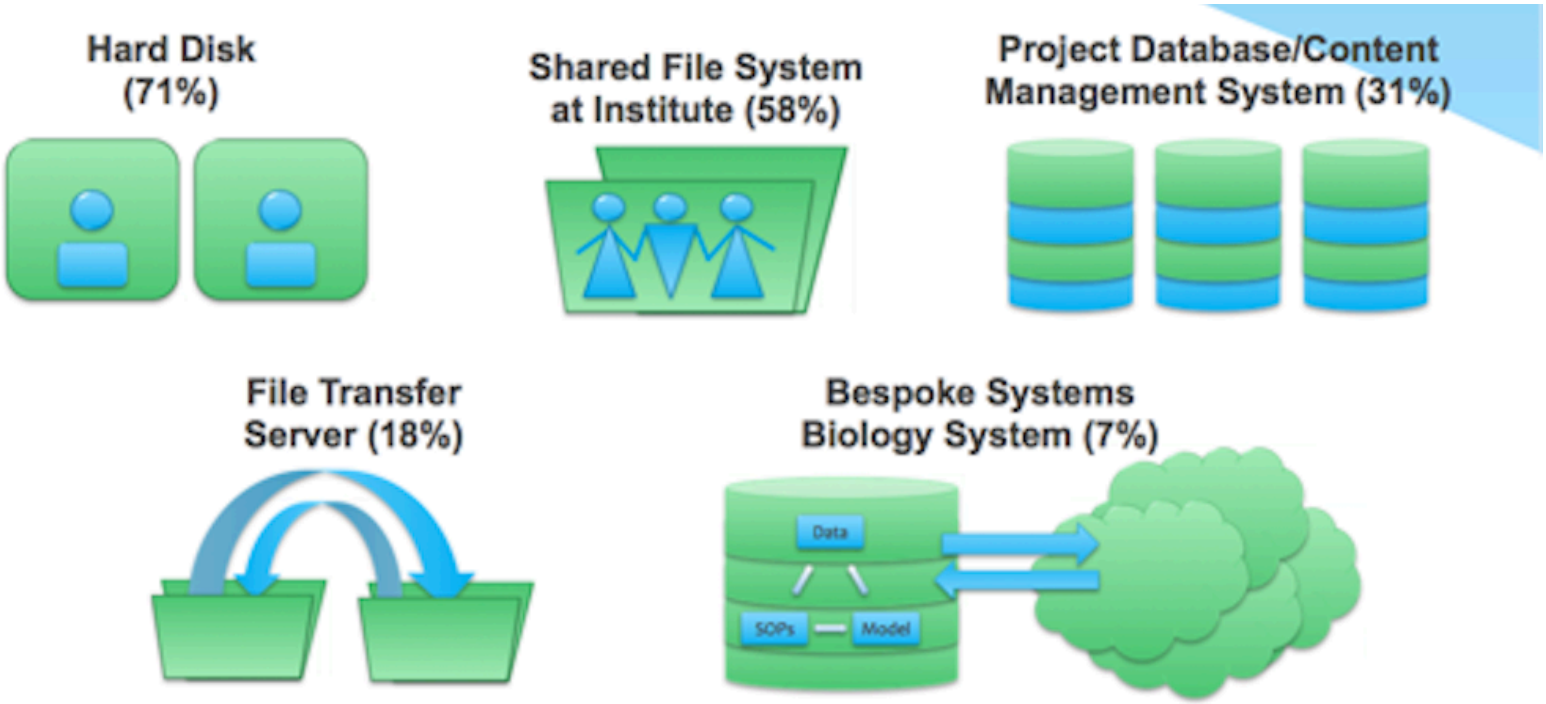
But how about storage and citing?

FINDABLE ??

ACCESSIBLE ??

HITS

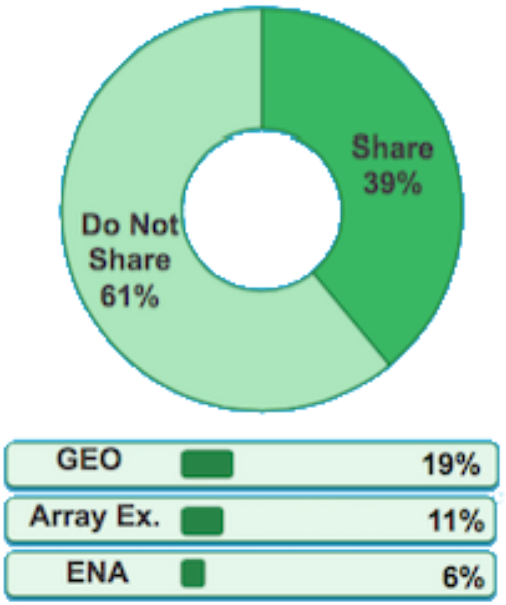
Researchers tend to store their data on their own hard disk



The evolution of standards and data management practices in systems biology (2015). Stanford, Wolstencroft, Golebiewski*, et al.*, Molecular Systems Biology, 11(12):851

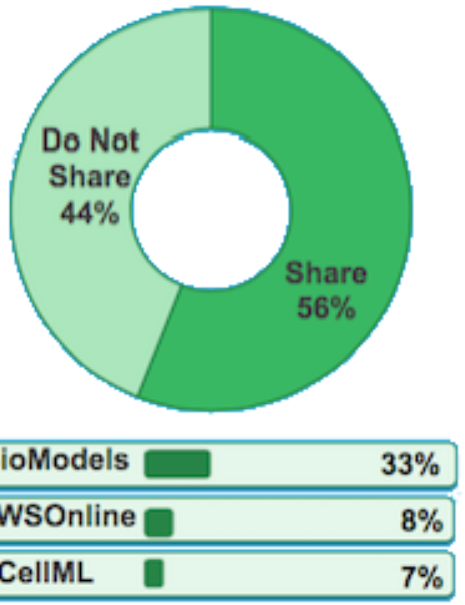
Many researchers do not share their data in open repositories.

Data



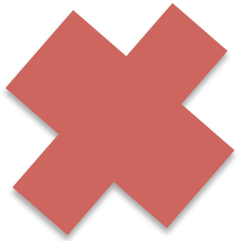
*top three most popular

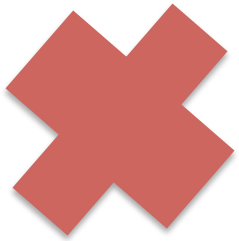
Models

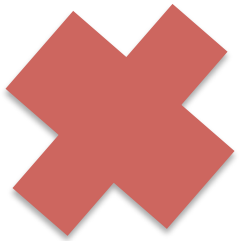


The evolution of standards and data management practices in systems biology (2015). Stanford, Wolstencroft, Golebiewski*, et al.*, Molecular Systems Biology, 11(12):851

This type of data management does not adhere to FAIR principles.

FINDABLE 

ACCESSIBLE 

REUSABLE 

HITS

The FAIRDOM Platform

Front end: Science Commons

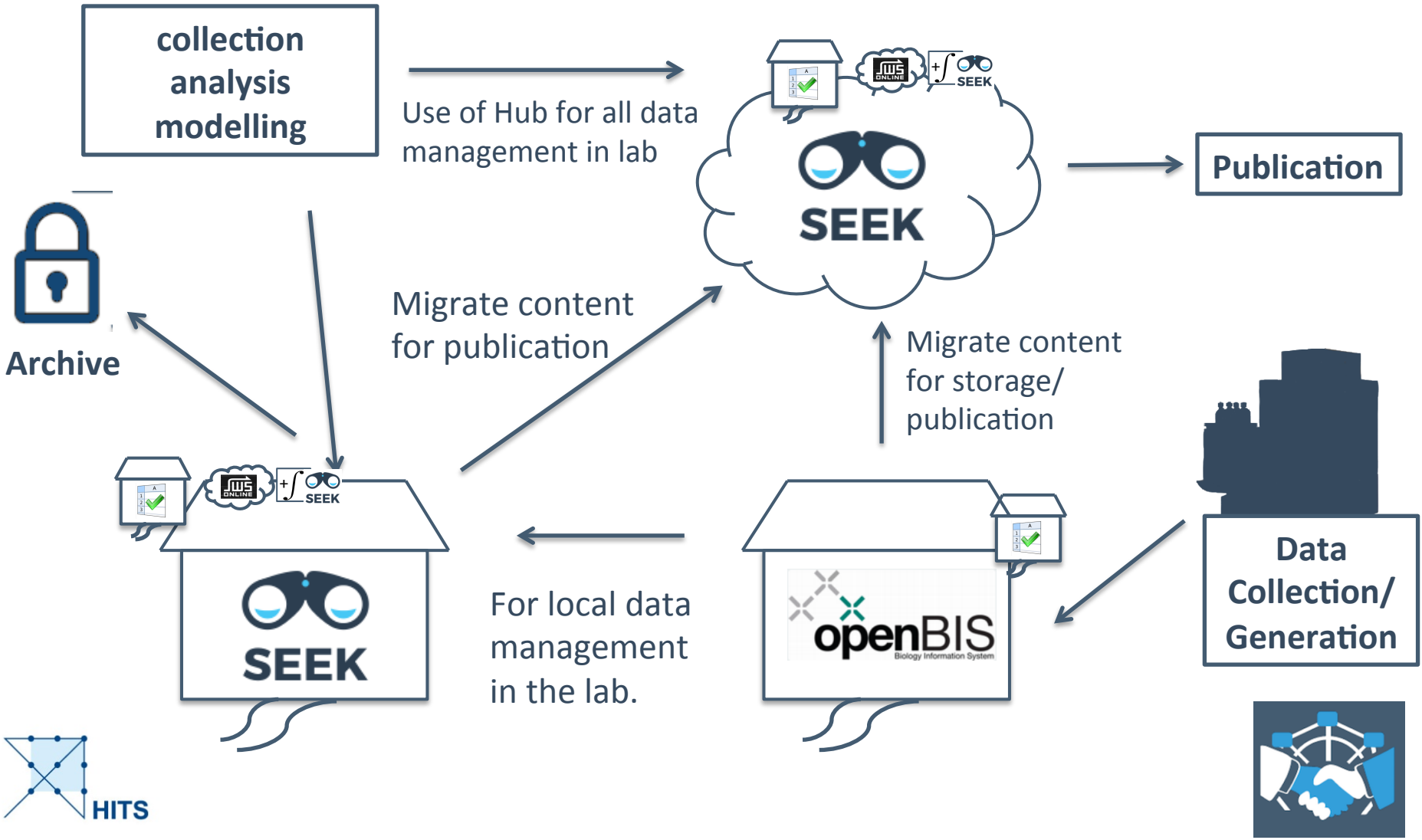
Web-based Cataloguing and Rich web interface for describing, finding, linking and promoting ongoing research and outcomes. Small files, aggregates across data archives.

Back end: Scaled local LIMS and analytics

Extract, Transform and Load tooling direct from the instrumentation, data analysis pipelines. Automatic archiving. Handles large data.

HITS

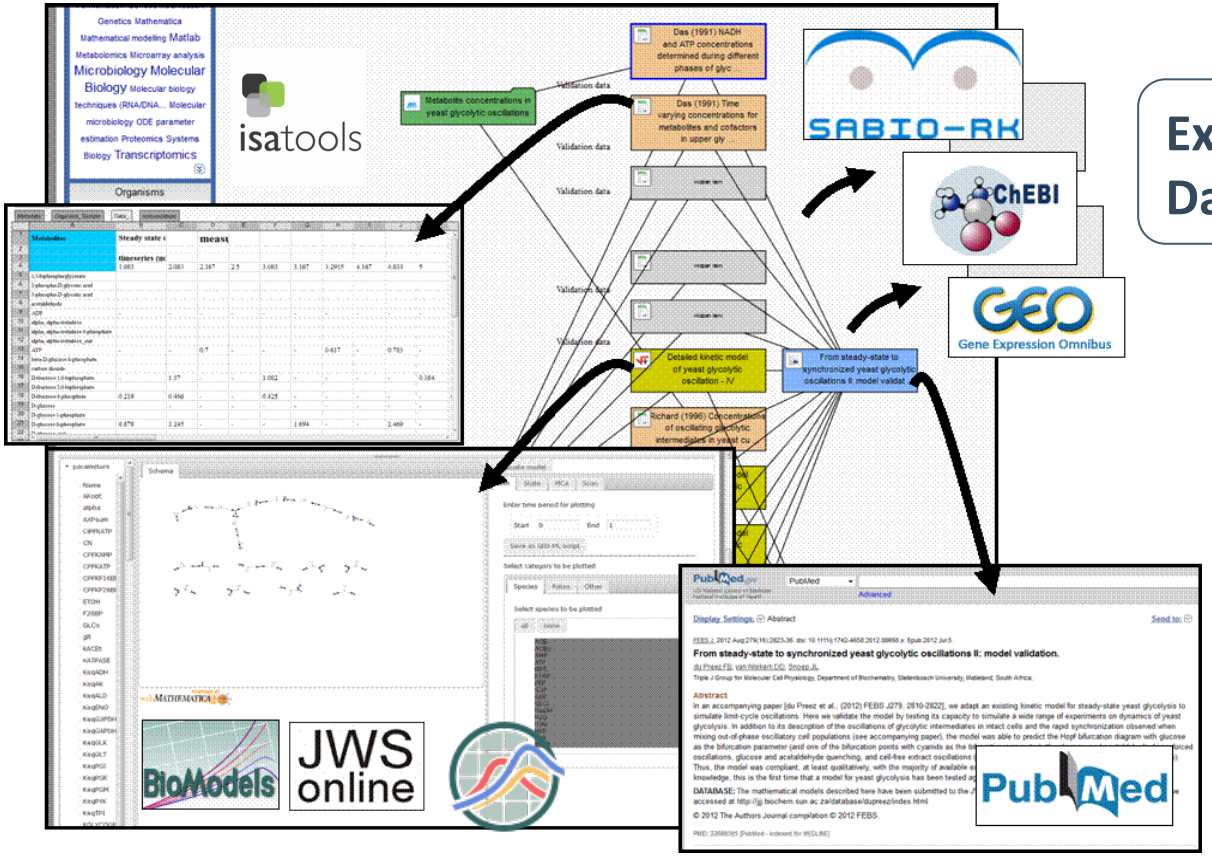
A typical use pipeline for a research group.



You can use SEEK as a local instance, or the FAIRDOMHub in the cloud.

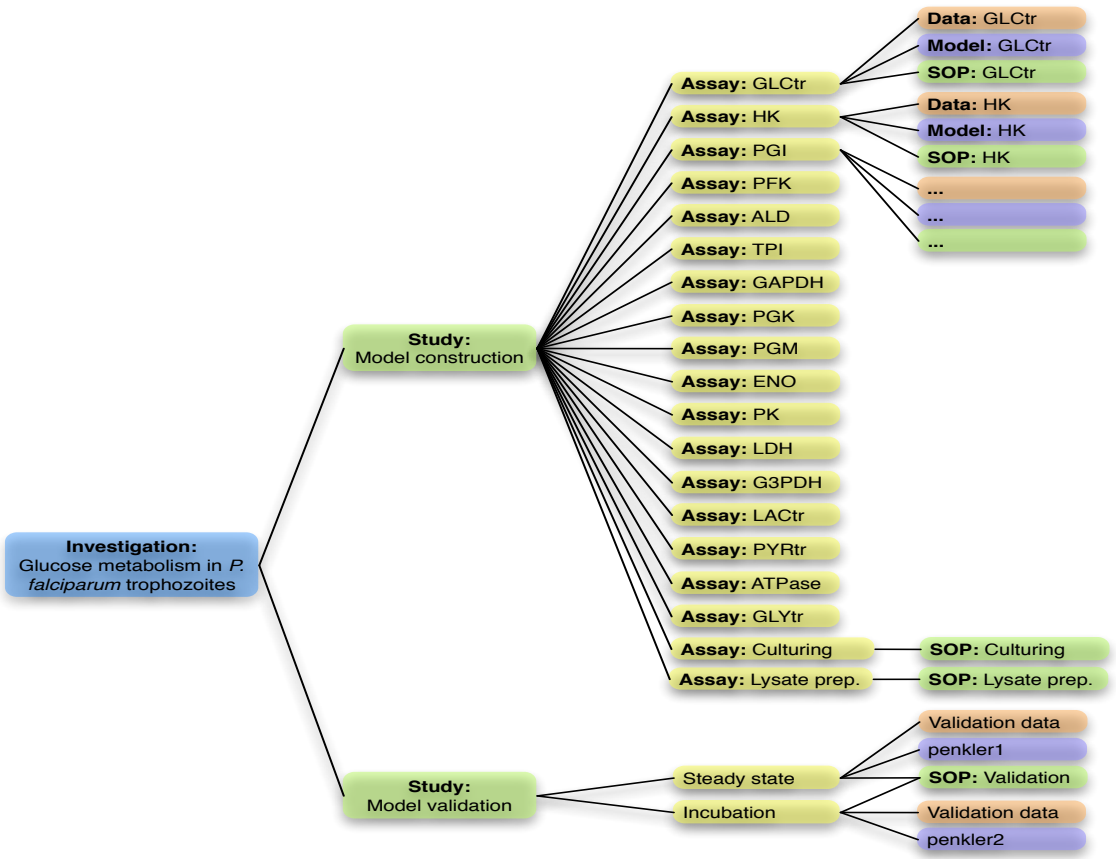
HITS

SEEK cross-relates and aggregates data, models, their metadata and related information



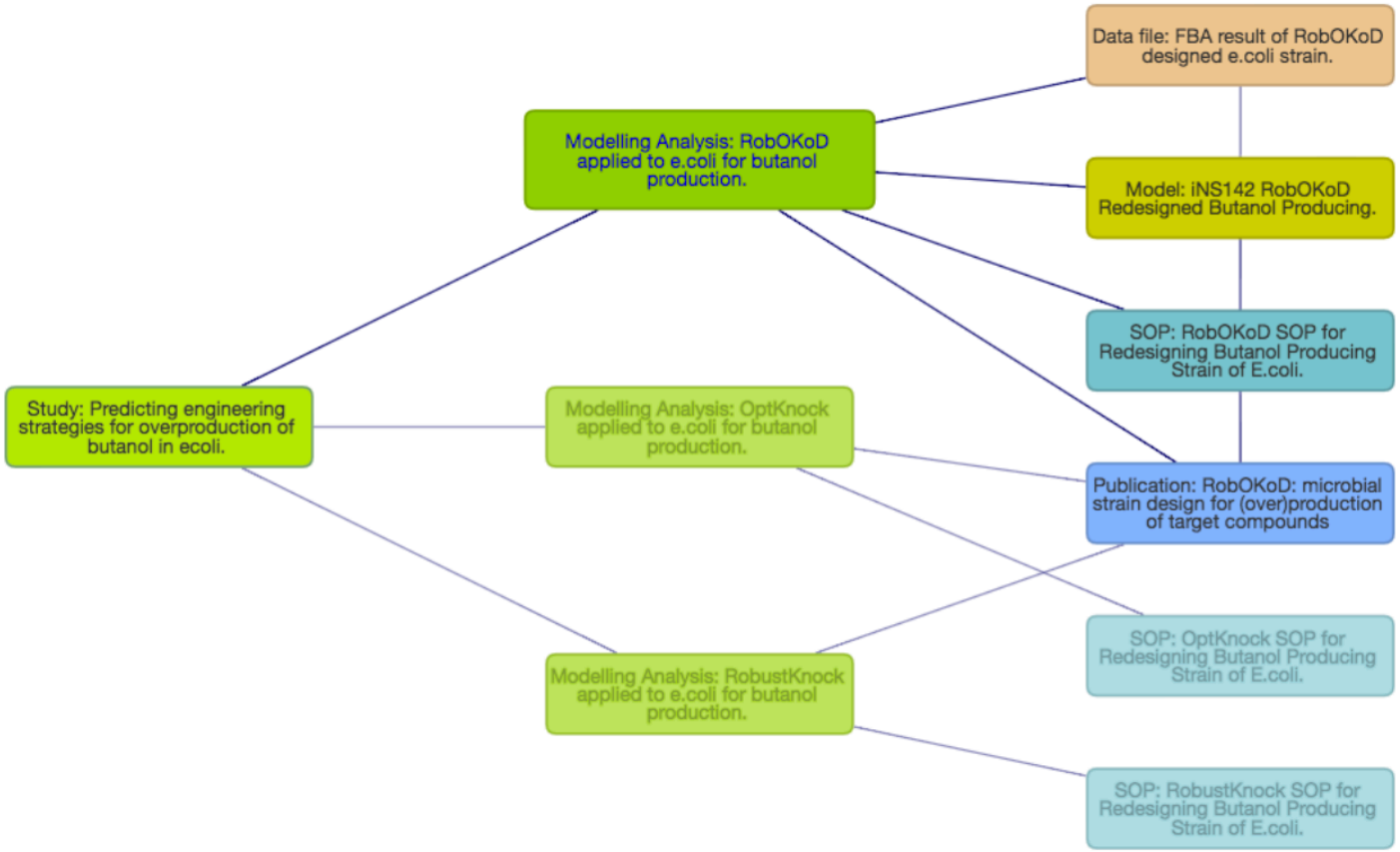
HITS

Structuring of data, metadata and files in an ISA (Investigation, Study, Assay) tree.



HITS

Selected item: Modelling Analysis: RobOKoD applied to e.coli for butanol production.



It has integrated support for SBML models

FAIRDOM Browse Create Help Search here... Search Natalie Stanford

Home / Models Index / Potato model

Potato model Version 3

Simulate Model on JWS | Subscribe | Download | Administration

No description specified

3 items are associated with this Model:

- assmus_third_version.xml (XML document - 83.5 KB)
- assmus_second_version.xml (XML document - 84.5 KB)
- assmus_original_version.xml (XML document - 84.9 KB)

Organism: *Not specified*

Model type: Ordinary differential equations

Model format: SBML

Execution or visualisation environment: JWS Online

Model image: *No image specified*

Contributors

License

No license specified
Click here to choose a license

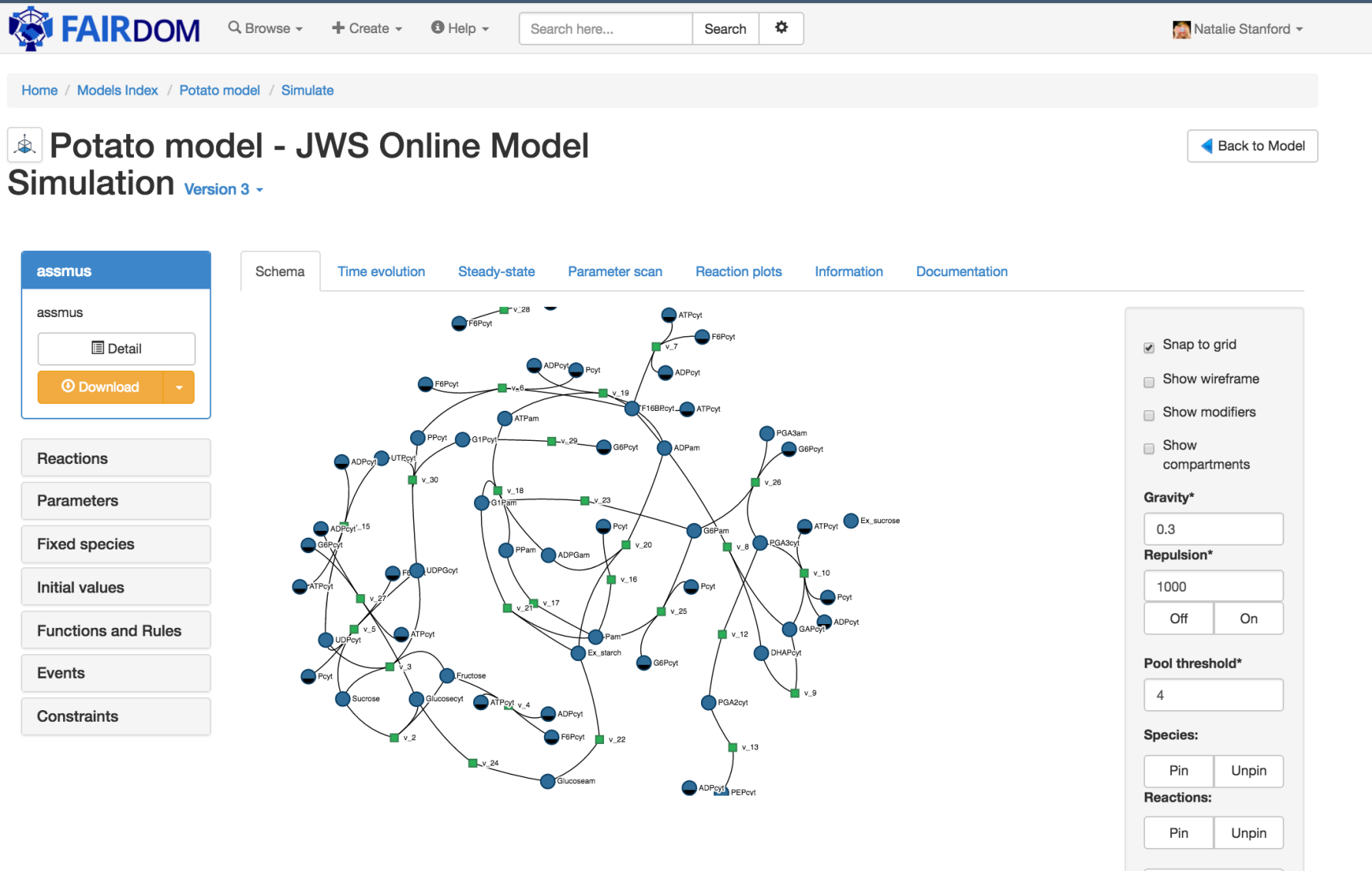
Activity

Views: 313 **Downloads:** 13

Created: 28th Oct 2015 at 17:54
Last updated: 29th Oct 2015 at 14:41
Last used: 16th Sep 2016 at 07:23

HITS

Integrated simulation with JWS Online



Comparison of version changes.

Deletions are coloured in red and insertions are coloured in blue

SBML Differences

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

Parameters

VappSPSSPP	Attribute ***value*** has changed: 797 → 500

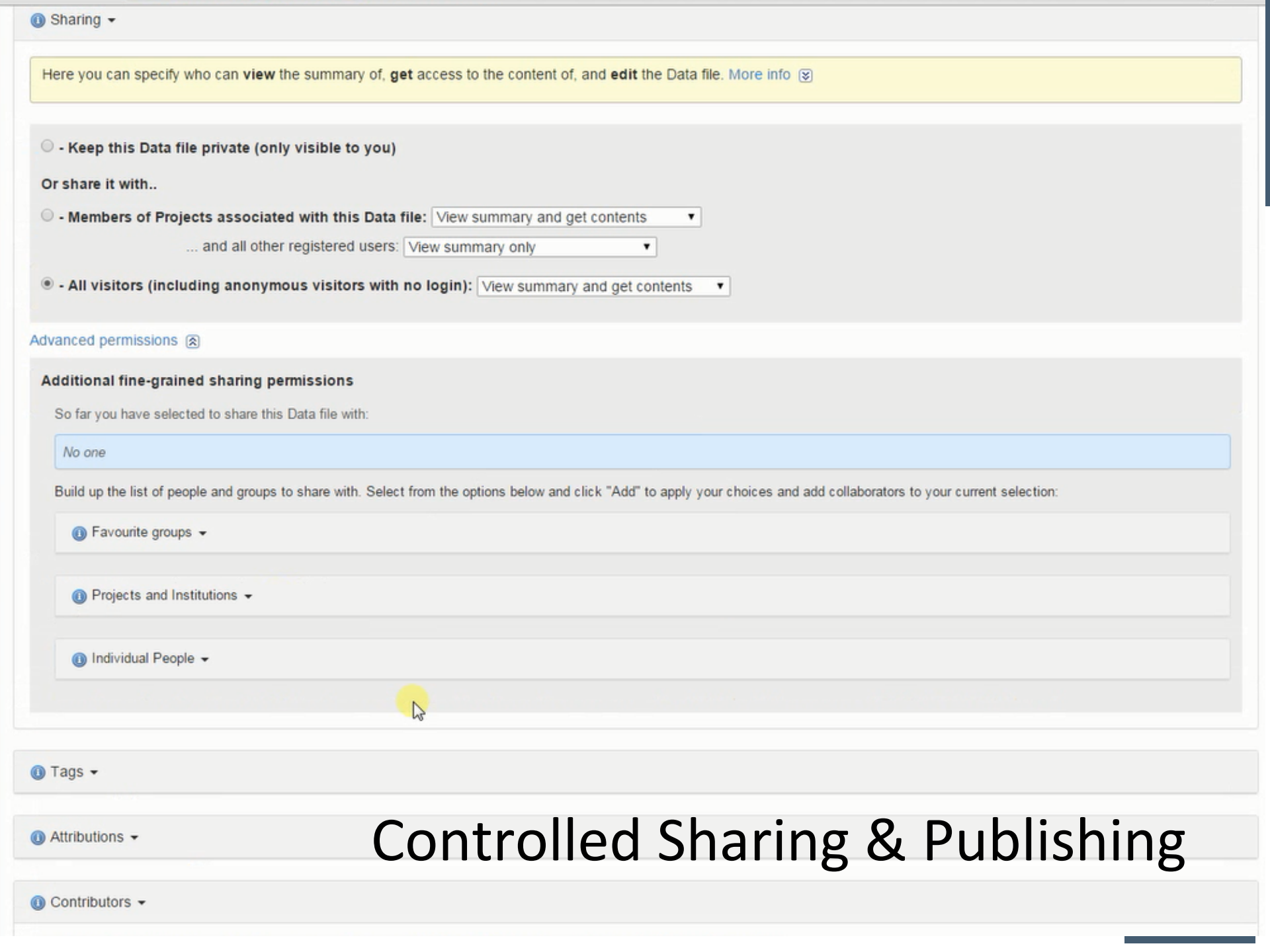
Compartments

default_compartment → main	Attribute ***id*** has changed: default_compartment → main

Species

Sucrose	Attribute ***compartment*** has changed: default_compartment → main
ADPGam	Attribute ***compartment*** has changed: default_compartment → main
PPam	Attribute ***compartment*** has changed: default_compartment → main
Pcyt	Attribute ***compartment*** has changed: default_compartment → main
F6Pcyt	Attribute ***compartment*** has changed: default_compartment → main
ADPam	Attribute ***compartment*** has changed: default_compartment → main
UDPcyt	Attribute ***compartment*** has changed: default_compartment → main
Glucoseam	Attribute ***compartment*** has changed: default_compartment → main
G6Pam	Attribute ***compartment*** has changed: default_compartment → main

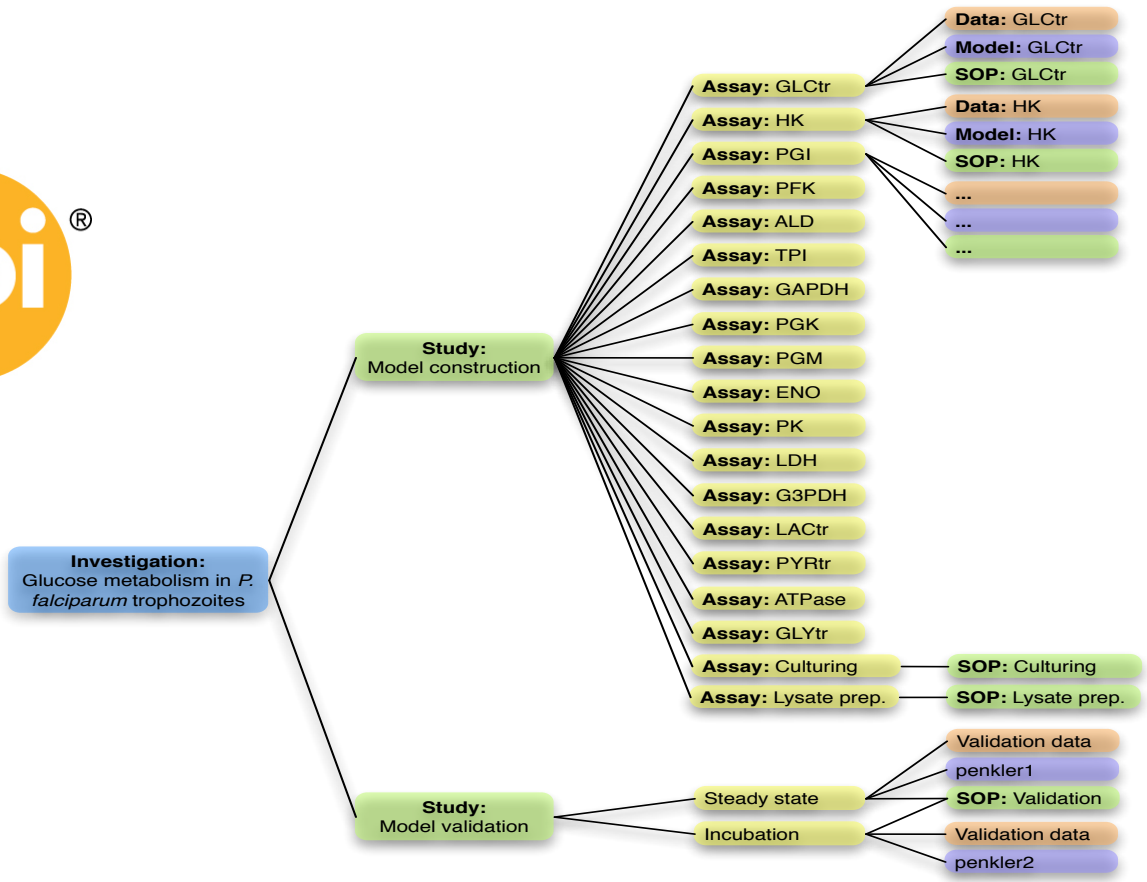
HITS


Sharing
Here you can specify who can view the summary of, get access to the content of, and edit the Data file. More info
- Keep this Data file private (only visible to you)
Or share it with..
- Members of Projects associated with this Data file: View summary and get contents
... and all other registered users: View summary only
- All visitors (including anonymous visitors with no login): View summary and get contents
Advanced permissions
Additional fine-grained sharing permissions
So far you have selected to share this Data file with:
No one
Build up the list of people and groups to share with. Select from the options below and click "Add" to apply your choices and add collaborators to your current selection:
Favourite groups
Projects and Institutions
Individual People
Tags
Attributions
Contributors
Controlled Sharing & Publishing

You can generate snapshots.

HITS

And assign DOIs to snapshots.



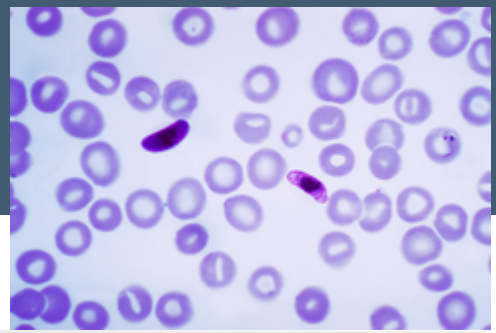
HITS

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]

1 Department of Biochemistry, Stellenbosch University, Matieland, South Africa
2 Molecular Cell Physiology, Vrije Universiteit Amsterdam, The Netherlands
3 MIB, University of Manchester, UK



https://doi.org/10.15490/seek.1.investigation.56

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

Correspondence
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(Received 19 August 2014, revised 7 February 2015, accepted 13 February 2015)

doi:10.1111/febs.13237

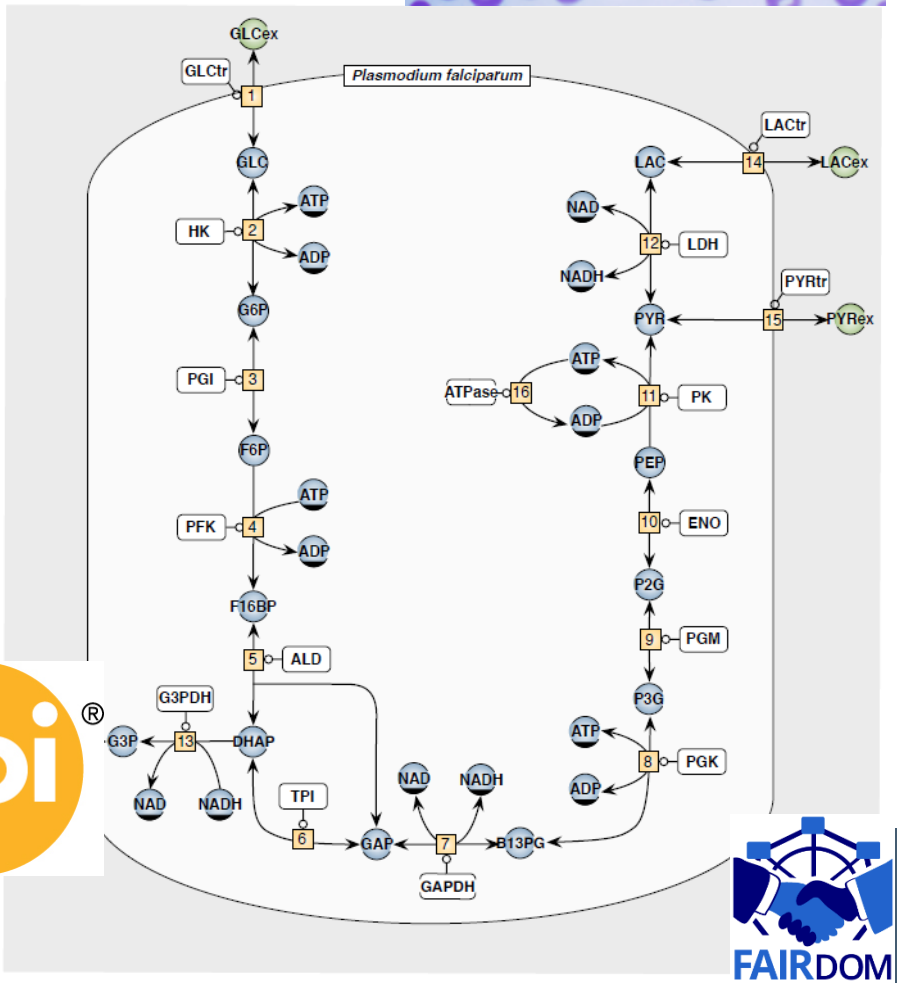
The enzymes in the Embden–Meyerhof–Parnas pathway of *Plasmodium falciparum* trophozoites were kinetically characterized and their integrated activities analyzed in a mathematical model. For validation of the model, we compared model predictions for steady-state fluxes and metabolite concentrations of 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).

Introduction

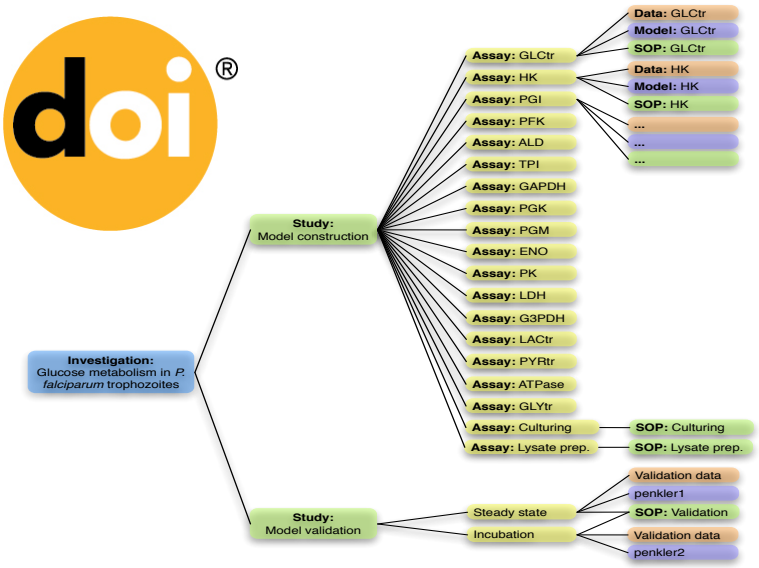
Despite several attempts at a complete eradication of the disease, malaria is still killing more than half a million people per year, mostly small children in sub-saharan Africa (World Health Organisation Malaria report 2013, http://www.who.int/malaria/publications/world_malaria_report_2013/en/). The 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, a

Abbreviations
2PG, 2-phosphoglycerate; 3PG, 3-phosphoglycerate; ALD, fructose-bisphosphate aldolase; B13PG, 1,3-bisphosphoglycerate glycerone phosphate; ENO, phosphopyruvate hydratase; F16BP, fructose 1,6-bisphosphate; F6P, fructose 6-phosphate; G3 3-phosphate; G3PDH, glycerol 3-phosphate dehydrogenase; G6P, glucose 6-phosphate; GAP, D-glyceraldehyde 3-phosphate glyceraldehyde 3-phosphate dehydrogenase; GLC, glucose; GLY, glycerol; HK, hexokinase; LAC, lactate; LDH, lactate dehy monocarboxylate transporter; ODE, ordinary differential equation; PEP, phosphoenolpyruvate; PFK, 6-phosphofructokinase; phosphate isomerase; PGK, phosphoglycerate kinase; PGM, phosphoglycerate mutase; PK, pyruvate kinase; PYR, pyruvate cell; TCA, tricarboxylic acid; TPI, triose-phosphate isomerase.



Penkler et al (2015) FEBSJ 282:1481-1511.

Research Objects allow for easy download and reuse.



HITS

FINDABLE ✔

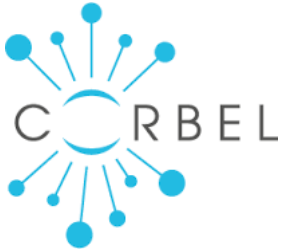
ACCESSIBLE ✔

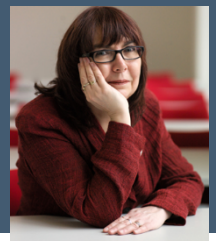
INTEROPERABLE ✔

REUSABLE ✔

HITS

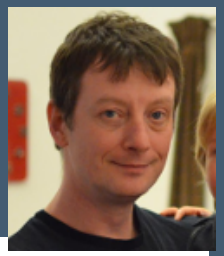
We are working and integrating with other initiatives to support this work.



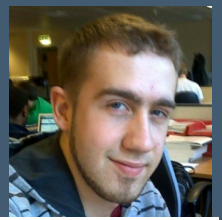


Carole Goble

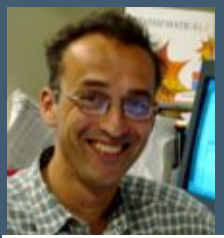
Natalie Stanford



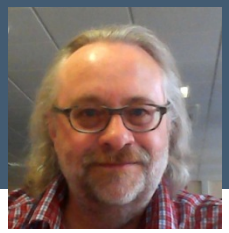
Stuart Owen



Finn Bacall



Jacky Snoep



Alan Williams

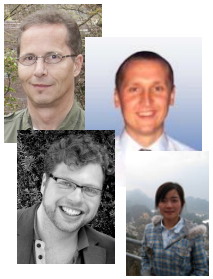
Wolfgang Mueller

Olga Krebs

Quyen Nguyen

Standards

Martin Golebiewski



Andrew Millar

Bernd Rinn

Lars Malmstroem

Rostyslav Kuzyakiv

Jakub Straszewski

Caterina Barillari

Jacky Snoep

Dawie van Niekerk

Katy Wolstencroft

Norman Morrison

Core Funders

FAIRDOM Usage

LiSyM
Liver Systems Medicine

de.NBI
GERMAN NETWORK FOR BIOINFORMATICS INFRASTRUCTURE

SynthSys
Centre for Synthetic and Systems Biology

SYNBIOCHEM

virtual liver network

SysMO
Systems Biology of Microorganisms

EMSL
Pacific Northwest
NATIONAL LABORATORY

Independent researchers

1000100 1010011
DIGITAL SALMON

RosAge
Reactive oxygen species and the dynamics of ageing

SBEpo

EVIMalaR

JENAGE
JENA CENTRE FOR SYSTEMS BIOLOGY OF AGEING
HITS

GenoSysFat

SulfoSYS biotec

LungSysII

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