



FAIRDOMHub for storing, finding, sharing, and reusing of data, models, operations

Olga Krebs

Heidelberg Institute for Theoretical Studies

EmPowerPutida project meeting and practical workshop on data management, Brussels, 30-23 November 2016



Agenda

- 40 minutes
 - What is data and model management ?
 - What do we offer?
- 40 minutes step by step powerpoint demo
- 40 minutes hands on
- Questions



Carole Goble



Jacky Snoep



Wolfgang
Mueller



Rostyslav
Kuzyakiv



Natalie
Stanford



Olga Krebs



Bernd Rinn



Stuart Owen



Quyen Nguyen



Katy Wolstencroft



also contributing:
UK SEEK team



also contributing:
SDBV team



FAIRDOM PALs

- Post-docs, Postgrads
 - **Co-designers,**
 - **Advocates**
 - Seed knowledge network
 - Bridge modellers-experimentalists
-
- Training
 - Workshops, meetings,
 - Kick-offs, Visits.....



FAIRDOM project funding



Bundesministerium
für Bildung
und Forschung



Funding set aside **independent of projects**

For centralized

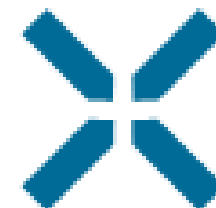
- Data&models management
- Services
- Community development
- Outreach





Experience with big project DMM

13 consortia
9 European countries
> 300 people



SystemsX.ch
The Swiss Initiative in System Biology



1 country
> 100 projects
> 300 groups

1 country
44 organisations
45 subprojects
> 250 people



ERASys APP
ERA-Net for Applied Systems Biology

12 consortia





DigiSal



Systems Science
for Health (SSfH)



Host-pathogen
interactions

SBCancer.

RosAge

Reactive oxygen species and
the dynamics of ageing



livSYSiPS



Consensus model
of Yeast Glycolysis





Findable
Accessible
Interoperable
Reusable

Data
S O P s
Models



Assets

<http://www.fair-dom.org>

<http://www.fairdomhub.org>



Why data management?

Data Sharing and Management Snafu in 3 Short Acts
by Karen Hanson, Alisa Surkis & Karen Yacobucci
NYU Health Sciences Libraries
August 3, 2012 (Last Update: December 12, 2012)



<https://scholarlykitchen.sspnet.org/2016/11/11/a-painful-but-true-to-life-look-at-data-availability-and-reuse/>





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.

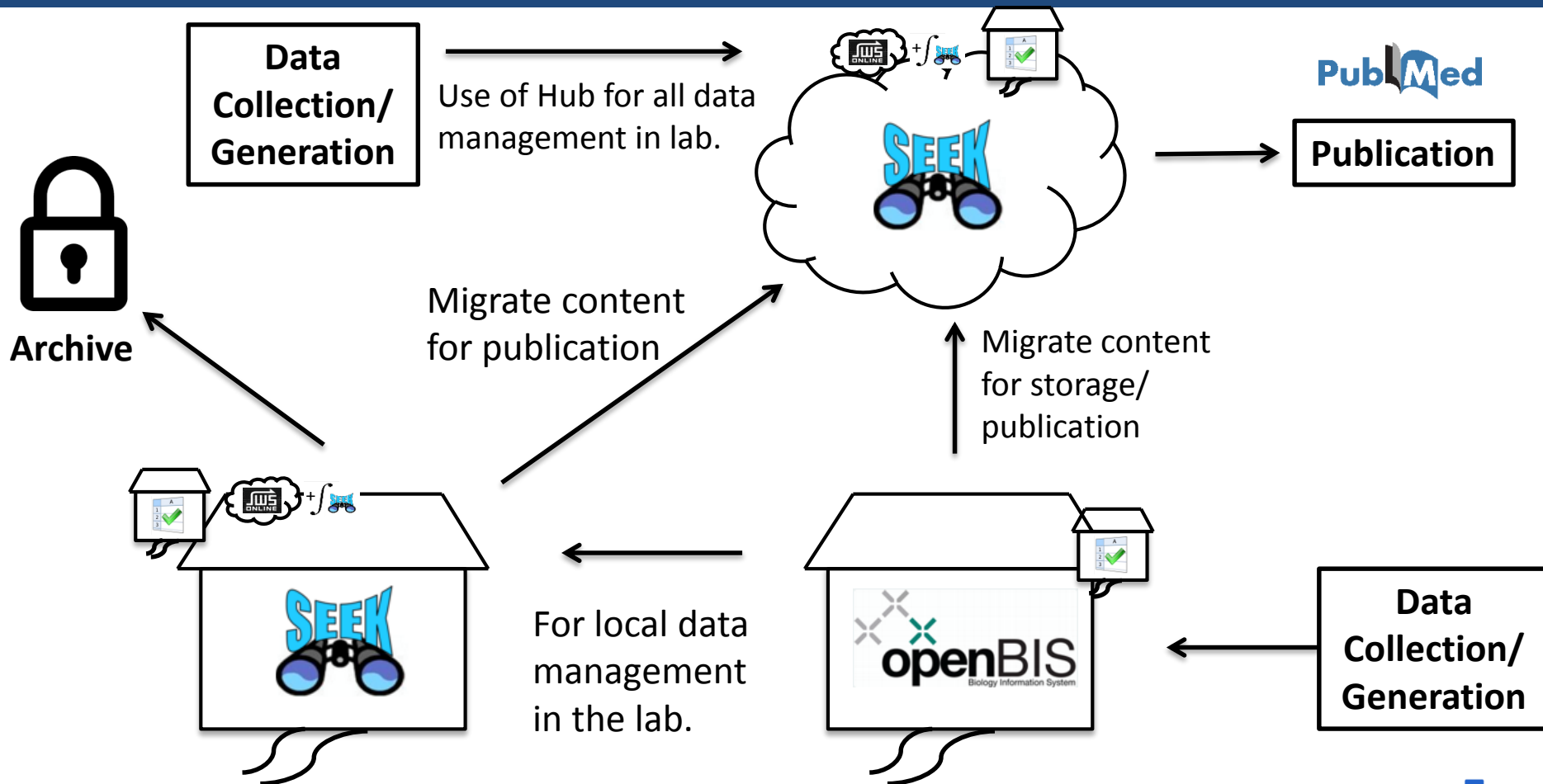


Back end: Scaled local Data Mgt. (incl. LIMS/ELN) and analysis integration

Ingest and transformation directly from the instruments or a web app, link with data analysis pipelines. Automatic archiving support. Very scriptable. Handles also large data.



How to use FAIRDOM





SEEK[illegible]

Personal Data Local Stores


Construction data:

Detailed kinetic model of yeast glycolytic oscillation - IV

Richard (1996) Concentration of oscillating glycolytic intermediates in yeast cu



Detailed kinetic model of yeast glycolytic oscillations

 Detailed kinetic model of yeast glycolytic

From steady-state to
synchronized yeast glycolytic
oscillations II: model validat ...

SOPs

Models

JWS
online



Articles



FAIRDOMHub: Platform Features

yellow pages
of peers
projects,
experts



project mgt,
access control
reporting, citation
governance &
policies



integrate local
tools and data
systems

catalogue and link
data, models,
samples, specimens,
sops, experiments,
publications using
standards



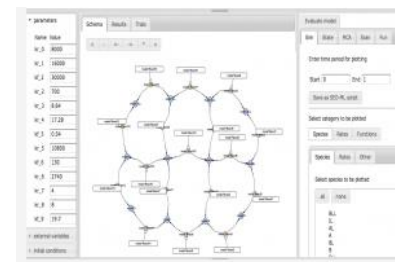
manage, store and
exchange different
types and scales
of data



access, link to and
deposit in public
data and model
repositories



simulate models

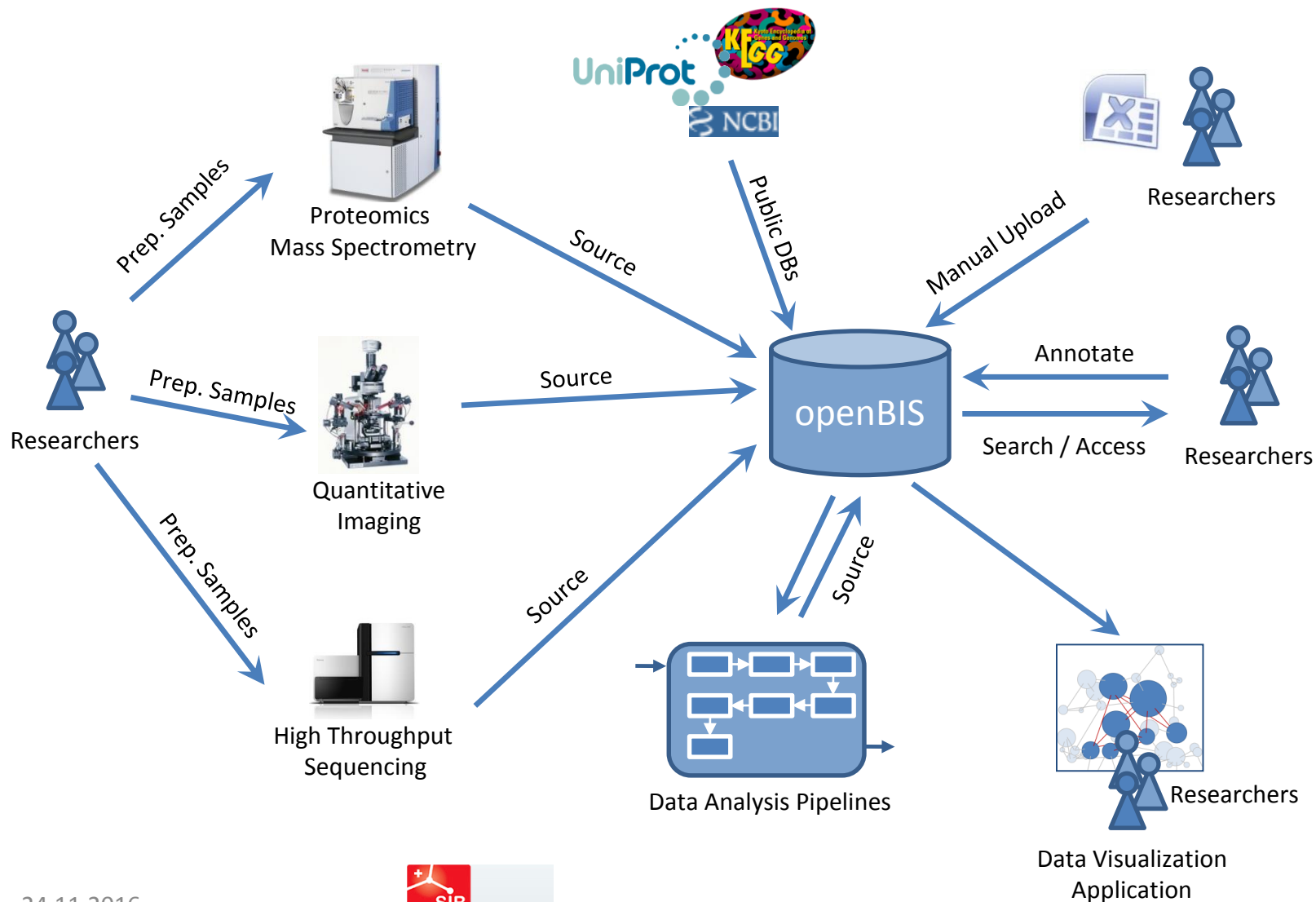


curate &
annotate data
and models
using standards



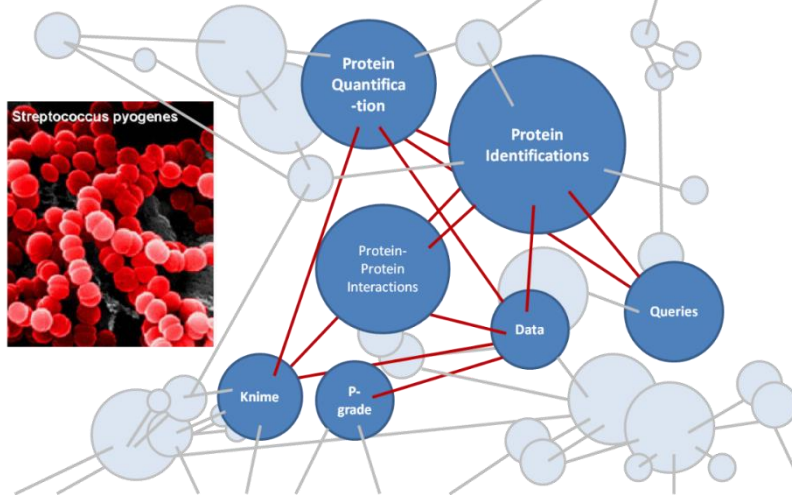
scaled-out collection & processing

openBIS in a nutshell

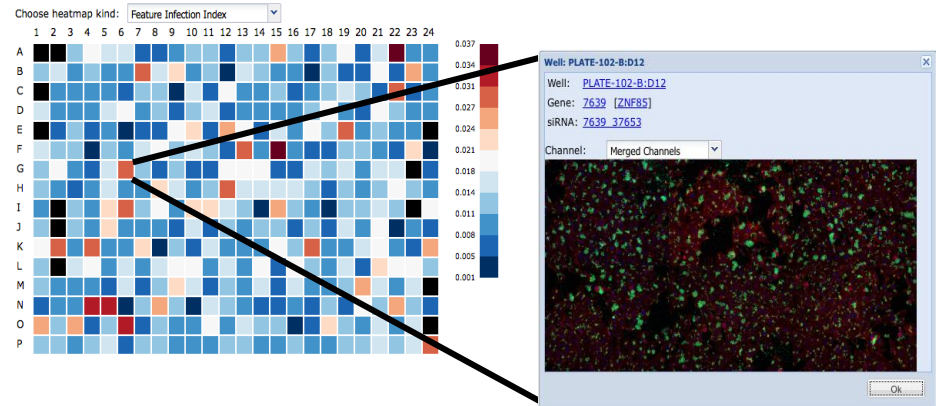


openBIS is used for...

Proteomics openBIS

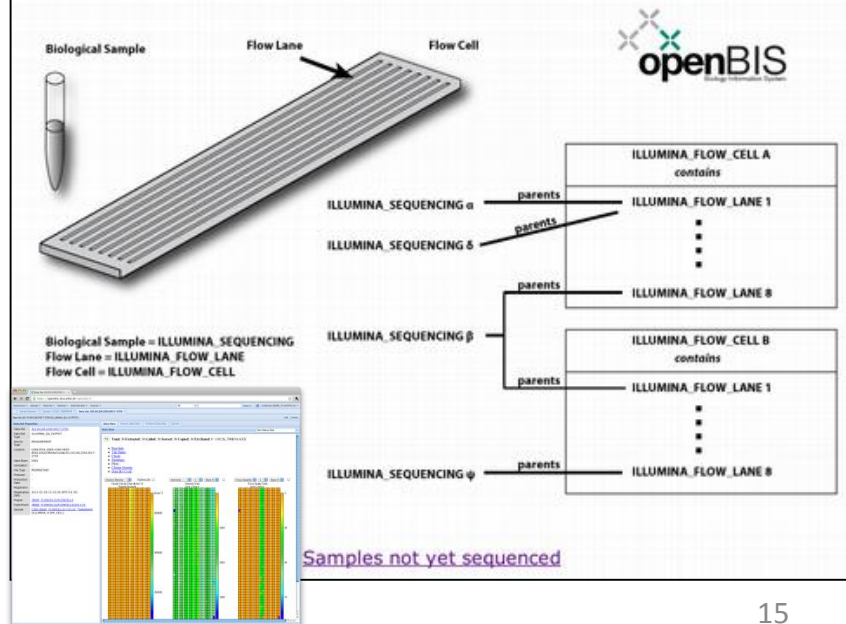


High Content Screening & Microscopy

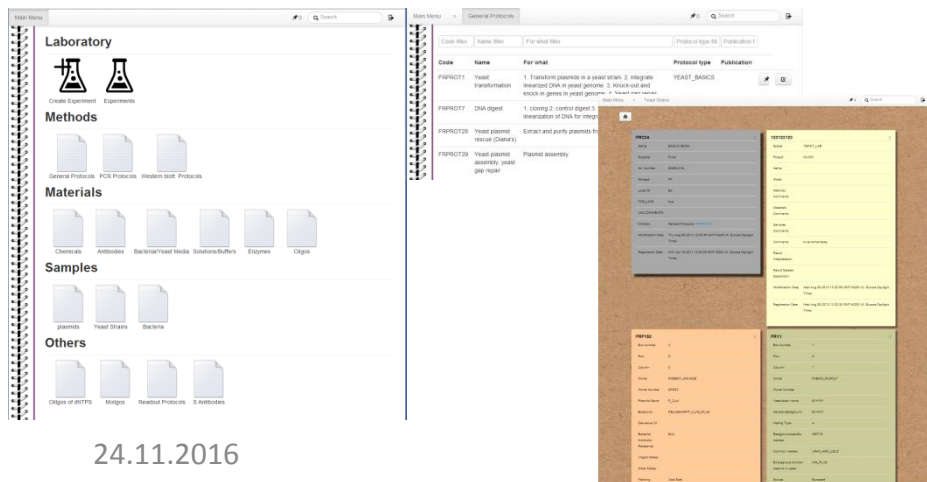


Next Generation Sequencing

Logical setup of the Deep Sequencing Unit (DSU) openBIS instance



Electronic Lab Notebook



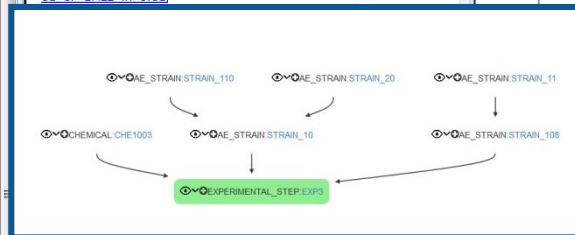
openBIS LIMS

metadata extraction
data relationship/linking
data processing
minimal user input

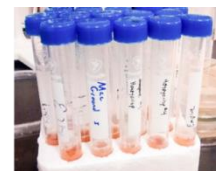
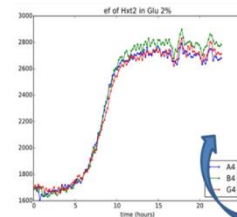
PS_GROUP » GROWTH_RATE » 187992378900 » PL13 » Data Set 187992378900 [PS_PLATE_READER]	
Data Set Properties	Data View
Sample	/PS_GROUP/PL13 [PS_IMG_PLATE]
Measurement date	2012-12-16
Measurement time	19:20:40
.mth file	March2012_2EmWL_1gain_M2_80c
Wsp file	2012_12_16.wsp
Instrument	infinite 200
Serial Nr	907001834
Plate desc.	[BD96ft_FluoroBlok] - BD Falcon 96 Flat Transparent/Black
Plate Cell Range	A1:H12
Temperature [C]	29.5
Min Temp. [C]	29.0
Max Temp. [C]	30.0
Shaking	Duration: 1000 sec; Mode: Linear; Amplitude: 6 mm; Frequency: 57.9 rpm;
Run Time	1days 45min 16s
Channels	OD 485-525mGain 485-585mGain
Channel1	OD Absorbance 595 nm reads:15
Channel2	485-525mGain

Folder:

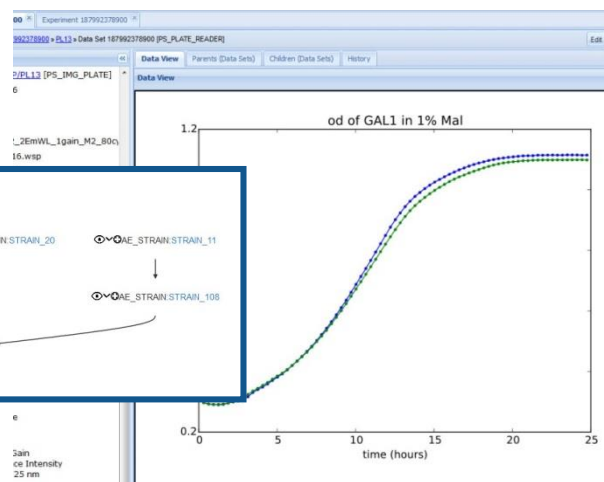
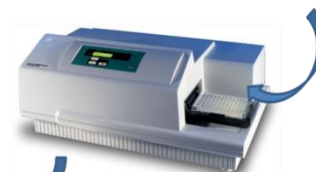
- 2012_12_16_GALgen
- GALgenes_contents
- od of GAL10 in 0.0
- od of GAL10 in 0.1
- od of GAL10 in 1p
- od of GAL10 in 2p
- od of GAL1 in 0.01
- od of GAL1 in 0.1p
- od of GAL1 in 1p
- od of GAL1 in 2p
- od of GAL2 in 0.01



od of GAL80 in 1p
od of GAL80 in 2p
od of null in 0.01p
od of null in 0.1p
od of null in 1p
od of null in 2p

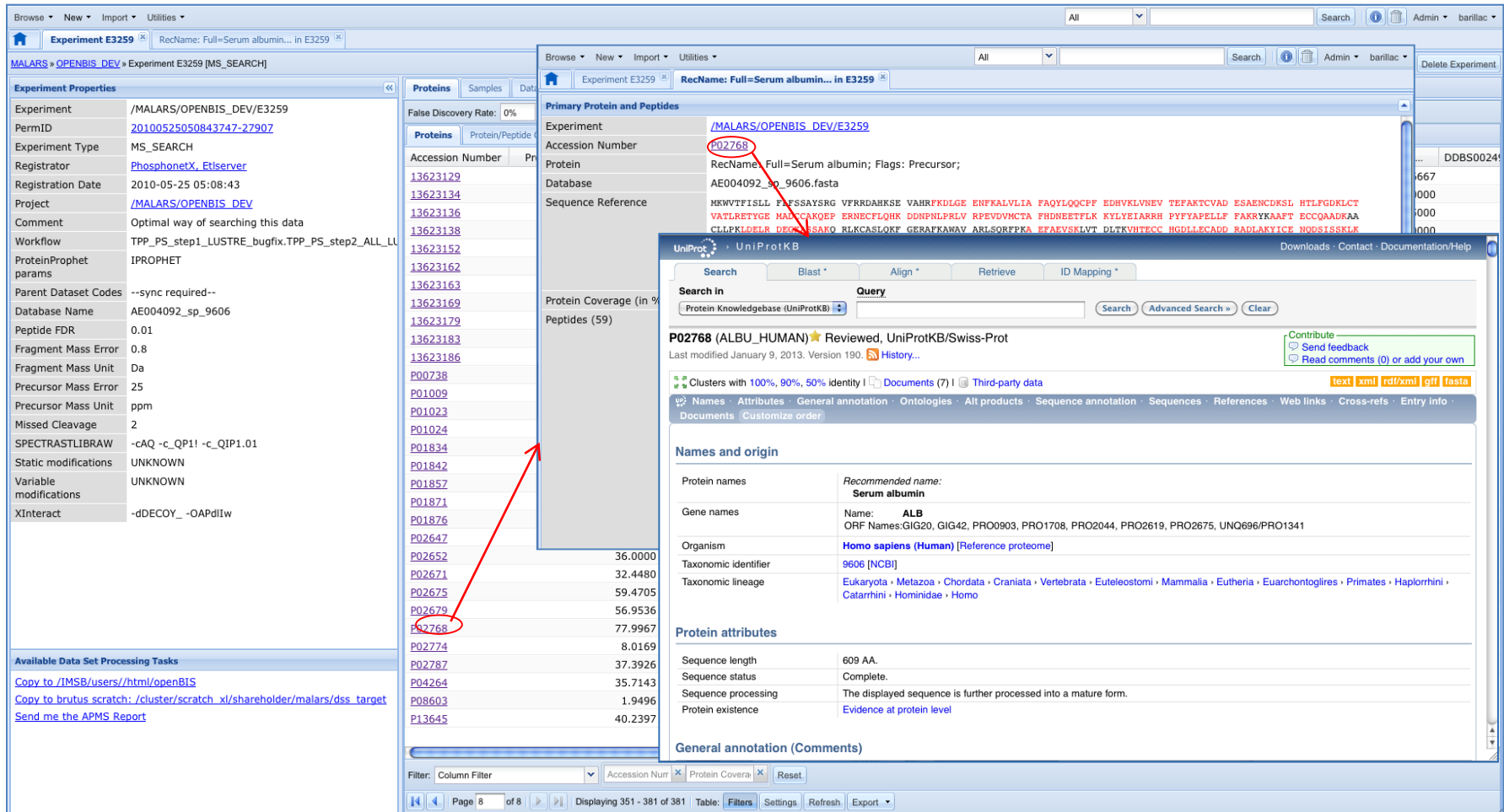


Time (h)	OD	Strain
0	1600	WT
1	1650	WT
2	1700	WT
3	1750	WT
4	1800	WT
5	1850	WT
6	1900	WT
7	1950	WT
8	2000	WT
9	2050	WT
10	2100	WT
11	2150	WT
12	2200	WT
13	2250	WT
14	2300	WT
15	2350	WT
16	2400	WT
17	2450	WT
18	2500	WT
19	2550	WT
20	2600	WT
21	2650	WT
22	2700	WT
23	2750	WT
24	2800	WT
25	2800	WT



openBIS : Platform for High-throughput Proteomics

Proteomics data in openBIS



The screenshot displays the openBIS platform interface for Experiment E3259. The left sidebar shows experiment properties, including the experiment name, type, registration date, and database name. The central table lists protein accessions and their corresponding protein coverage. The right panel provides detailed information for the selected protein, P02768 (ALBU_HUMAN), including its name, gene names, organism, and protein attributes.

Experiment Properties

- Experiment: /MALARS/OPENBIS_DEV/E3259
- PermID: 20100525050843747-27907
- Experiment Type: MS_SEARCH
- Registrar: PhosphonEX_Etlserver
- Registration Date: 2010-05-25 05:08:43
- Project: /MALARS/OPENBIS_DEV
- Comment: Optimal way of searching this data
- Workflow: TPP_PS_step1_LUSTRE_bugfix.TPP_PS_step2_ALL_LU
- ProteinProphet params: IPROPHET
- Parent Dataset Codes: --sync required--
- Database Name: AE004092_sp_9606
- Peptide FDR: 0.01
- Fragment Mass Error: 0.8
- Fragment Mass Unit: Da
- Precursor Mass Error: 25
- Precursor Mass Unit: ppm
- Missed Cleavage: 2
- SPECTRAL LIBRARY: -cAQ -cQP1 -c_QIP1.01
- Static modifications: UNKNOWN
- Variable modifications: UNKNOWN
- XInteract: -dDECOY_ -OAPdIw

Protein Coverage (in % Peptides (59))

Accession Number	Protein/Peptide	Protein Coverage (in % Peptides (59))
13623129		
13623134		
13623136		
13623138		
13623152		
13623162		
13623163		
13623169		
13623179		
13623183		
13623186		
P00738		
P01009		
P01023		
P01024		
P01834		
P01842		
P01857		
P01871		
P01876		
P02647		
P02652		36.0000
P02671		32.4480
P02675		59.4705
P02679		56.9536
P02768		77.9967
P02774		8.0169
P02787		37.3926
Q04264		35.7143
P08603		1.9496
P13645		40.2397

Primary Protein and Peptides

Experiment: /MALARS/OPENBIS_DEV/E3259
 Accession Number: P02768
 Protein: RecName: Full=Serum albumin; Flags: Precursor;
 Database: AE004092_sp_9606.fasta
 Sequence Reference: MKWVTFISLL FAFSSAYSRG VFRRDAHSE VAHRFDLGE ENFKALVLA FAQYLQCPFF EDHVKLVNEV TEFARTCVAD ESAENCDSKL HTLFGDKLCT VATLRETYGE MALCCAKQEP ERNECFLOHK DNPPLPLRV RPEVDNMCTA FHDNEETFLK KYLVEIARRH PYFYAPELFL FAKRYKAAFT ECGQAADKAA CLTPKLDGLR DEQSSAKO RLKCSLSQKF GERAFAKAW ARLSORFPKA EFAVEVSLVT DLTKVHTECC NGDLLECCAD RADLAKYICE NODSISSEKL

UniProtKB - UniProtKB

Search in: Protein Knowledgebase (UniProtKB) Query: [Search] [Advanced Search] [Clear]

P02768 (ALBU_HUMAN) Reviewed, UniProtKB/Swiss-Prot
 Last modified January 9, 2013. Version 190. [History...]

Clusters with 100%, 90%, 50% identity | Documents (7) | Third-party data
 [text] [xml] [rdf/xml] [gff] [fasta]

Names · Attributes · General annotation · Ontologies · Alt products · Sequence annotation · Sequences · References · Web links · Cross-refs · Entry info · Documents (Customize order)

Names and origin

Protein names	Recommended name:
Gene names	Serum albumin Name: ALB ORF Names: GIG20, GIG42, PRO0903, PRO1708, PRO2044, PRO2619, PRO2675, UNQ696/PRO1341
Organism	Homo sapiens (Human) [Reference proteome]
Taxonomic identifier	9606 [NCBI]
Taxonomic lineage	Eukaryota · Metazoa · Chordata · Craniata · Vertebrata · Euteleostomi · Mammalia · Eutheria · Euarchontoglires · Primates · Haplorhini · Catarrhini · Hominoidea · Homo

Protein attributes

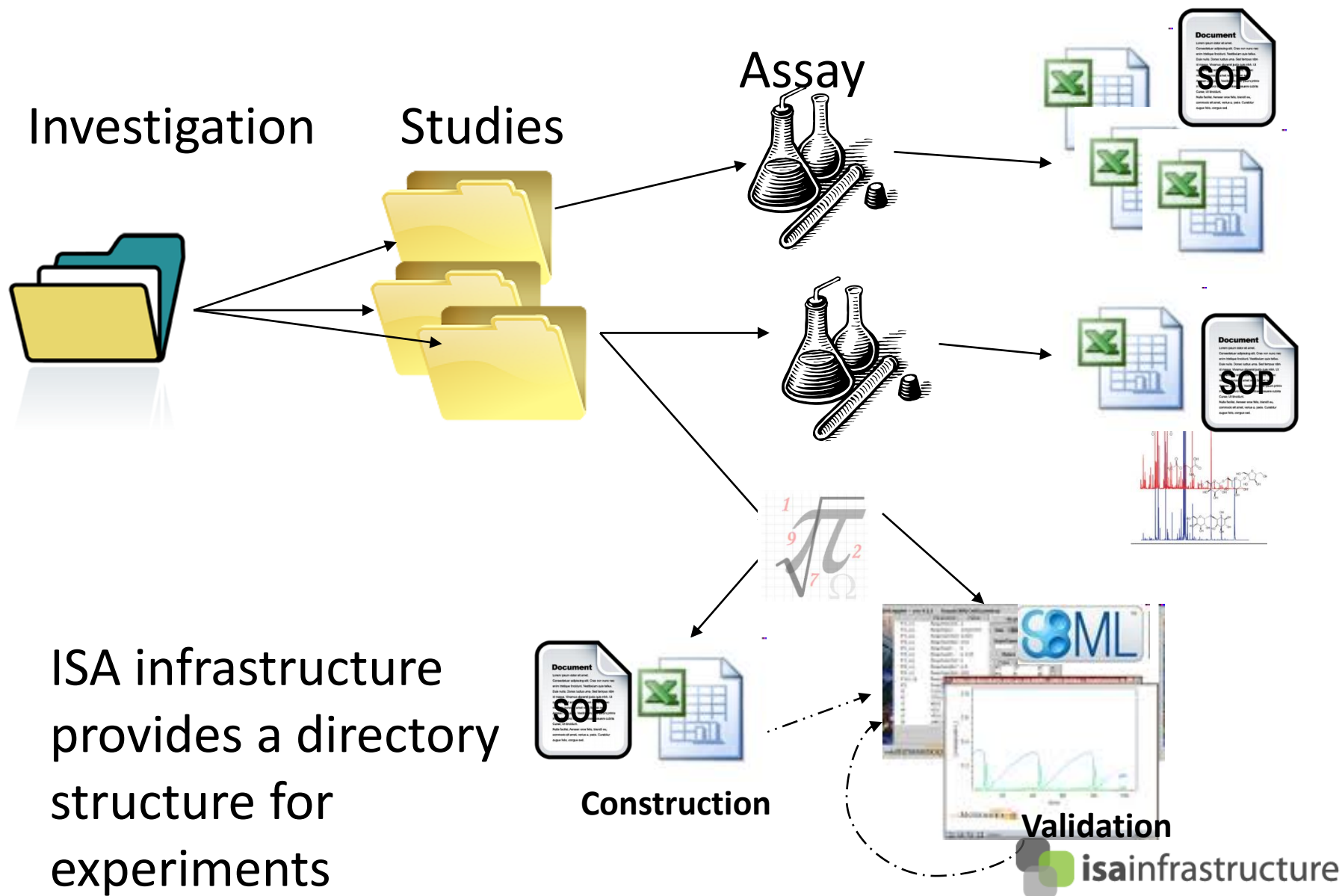
Sequence length	609 AA.
Sequence status	Complete.
Sequence processing	The displayed sequence is further processed into a mature form.
Protein existence	Evidence at protein level

General annotation (Comments)

Filter: Column Filter [x] Accession Num [x] Protein Covera [x] [Reset]

Page 8 of 8 | Displaying 351 - 381 of 381 | Table: [Filters] [Settings] [Refresh] [Export]

Organising and Linking Assets



....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 Plasmodium falciparum

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

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

Metadata	Values (examples)
Asset Title	PFK Kinetic Data
Uploader	David van Niekerk
Tglower SEED ID	
Project	
ASSAY	
Assay SEED ID	0
Assay Type	PFK
Assay Type	metabolic assay
Assay Type	metabolic assay
Description	kinetic characterisation of PFK, Enzyme
Experimentation	Enzyme
Date	
SOP	Publication (optional)
Publication (optional)	
Experimental conditions	
Incubation	temperature
Composed of (concentration)	ATP
Unit	°C
Start_value (optional)	37
End_value (optional)	37
Comments	
Culture growth	Batch
FACTORS STUDIED	
Incubation	concentration
Composed of (concentration)	ATP
Unit	mol
Start_value (optional)	0
End_value (optional)	10
Comments	

Analysis (Assay)

PFK SOP:

Specific activity of the glycolytic enzymes were measured in NAD(P)H-dependent linked enzyme assays that were adapted from Teusink et al. (11) and measured at 340 nm in 96-well plates (Flat Bottom microplate, Greiner Bio-One, Kremsmünster, Austria) on a spectrophotometer (MicroScan microplate reader, Thermo Electron Corporation, Waltham, Massachusetts, USA). The same buffer, (20 mM HEPES, 20 mM MgCl₂, 10 mM KCl and 10 mM NaCl), was used for all assays, with a pH set to 7.17, matching the cytosolic pH of *P. falciparum* (12) (13). 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 acyl-P_{CoA}, ADL, TPL. Product inhibition by F6BP (0 - 60 mM) was assayed by linking the production of ADP to the oxidation of NADH (0.8 mM) via LPL. PK in the presence of PFK (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.

(11) Teusink B, Passarge J, Reijnders C, Eggink G, 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: 5313-5325.

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

Data

Data file: PFK Kinetic data

Model

Model: PFK Kinetic model

SOP

PFK Kinetic model

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

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

- PFK-SEEK.nb (Mathematica Notebook - 203 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)

$$v_{PFK} = \frac{V_{PFK} \cdot \frac{atp}{K_{ATP}} \cdot \frac{f6p}{K_{F6P}}}{\left(1 + \frac{atp}{K_{ATP}}\right) \cdot \left(1 + \frac{f6p}{K_{F6P}} + \frac{f6bp}{K_{F6BP}}\right) \cdot \left(1 + \frac{atp}{K_{ATP}} + \frac{adp}{K_{ADP}}\right)}$$

Selected item: Model: PFK Kinetic model



FAIRDOMHub: Landing page

Welcome to SEEK

For information about FAIRDOM please visit our [FAIRDOM site](#).

For more information about the SEEK software and to see a video, please visit our [SEEK site](#).

SEEK News

FAIRDOM at ISMB 2015

FAIRDOM feed - 4 days ago

2015 Workshop on the Cardiac Electrophysiology Web Lab

FAIRDOM feed - about 1 month ago

ICSB 2015 will now be held in Singapore in November

FAIRDOM feed - about 1 month ago

COMBINE 2015

FAIRDOM feed - about 1 month ago

16th International Conference on Systems Biology 2015

FAIRDOM feed - about 1 month ago

Community News

Validation and selection of ODE based systems biology models: how to arrive at more reliable decisions

BMC Systems Biology - Latest Articles - 2 days ago

Modeling credentials

Nature Biotechnology - Issue - nature.com science feeds - 3 days ago

Genome in a bottle—a human DNA standard

Nature Biotechnology - Issue - nature.com science feeds - 3 days ago

GINA and the 'devious defecator' case

Nature Biotechnology - Issue - nature.com science feeds - 3 days ago

Gilead wades into epigenetics

Latest additions

Supply demand analysis on penkler1 model

Model - added about 3 hours ago

Supply-demand analysis

Modelling analysis - added about 3 hours ago

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

Publication - added about 22 hours ago

Description of data sets and protocol SARS-CoV siRNA screens human kinome

Data file - added 2 days ago

Latest downloads

[FAIRDH Kinetic data](#)

Data - downloaded about 1 hour ago

test doi with fairdomhub site base url

Data file - downloaded about 1 hour ago

MetApp - Zurich 6 month meeting - Jean-Charles

Data file - downloaded about 6 hours ago

Marta: meeting in Zurich

Data file - downloaded about 6 hours ago

Marta: meeting in Barcelona

Tags [show all](#)

[Bacillus subtilis](#) [Biochemistry](#) [Biochemistry and protein analysis](#) [Bioinformatics](#) [Computational and theoretical biology](#) [Computational Systems Biology](#) [Data Management](#) [Dynamic modelling](#) [dynamics and control of biological ne...](#) [Fermentation](#) [Genetic modification](#) [Genetics](#) [Mathematica](#) [Mathematical modelling](#) [Matlab](#) [Metabolomics](#) [Microarray analysis](#) [Microbiology](#) [Molecular Biology](#) [Molecular biology techniques \(RNA/DNA...\)](#) [ODE parameter estimation](#) [Proteomics](#) [Systems Biology](#) [Transcriptomics](#)

Organisms

- [Acidithiobacillus caldus](#)
- [Bacillus subtilis](#)
- [Chikungunya virus](#)
- [Clostridium acetobutylicum](#)
- [Coxsackievirus](#)
- [Dengue virus](#)
- [Enterococcus faecalis](#)
- [Escherichia coli](#)
- [Escherichia coli K-12](#)
- [Hepatitis C virus](#)
- [Homo sapiens](#)
- [Lactic Acid Bacteria](#)
- [Lactobacillus plantarum](#)
- [Lactococcus lactis](#)
- [Leptospirillum ferriphilum](#)
- [Mus musculus](#)
- [Plasmodium falciparum](#)
- [Pseudomonas fluorescens](#)
- [Pseudomonas putida](#)

FAIRDOMHub: Landing page

The screenshot shows the FAIRDOMHub landing page. The top navigation bar includes the FAIRDOM logo, a 'Browse' dropdown, a 'Create' dropdown, a 'Help' dropdown, and a search bar. A red arrow points from the 'Help' dropdown in the top bar to a larger, detailed 'Help' dropdown menu on the right. Another red arrow points from the 'Create' dropdown in the top bar to a detailed 'Create' dropdown menu on the right. The main content area features a 'FAIRDOMHub' header, a description of the initiative, and a list of categories on the left. The 'FAIRDOM News' section at the bottom left highlights recent events and webinars.

FAIRDOM

Q Browse ▾ + Create ▾ ⓘ Help ▾ Search here

FAIRDOMHub

The **FAIRDOMHub** is built upon a software suite, which is an open platform for sharing scientific assets, processes and outcomes. For more information about SEEK please visit <http://seek4science.com>

FAIRDOM is an initiative to develop a community, and establish an international Data and Model Management network to the European Systems Biology community. FAIRDOM is a joint action of the [A-Net EraSysAPP](#) and European Research Infrastructure [ISBE](#). For more information about FAIRDOM please visit <http://fair-dom.org>

Yellow pages

- Programmes
- People
- Projects
- Institutions
- Experiments
- Investigations
- Studies
- Assays
- Assets
- Data files
- Models
- SOPs
- Publications
- Activities
- Presentations

FAIRDOM News

[Summer school on Computational Biology](#)
FAIRDOM - Events - 3 days ago

[Miss out on our third webinar?](#)
FAIRDOM - 20 days ago

Primary sex chromosome study uncovers formation of sex chromosomes
Most Recent Art

Help

- Help documents
- Feedback
- Provide feedback

+ Create ▾ ⓘ

- Assets
- Data file
- Model
- SOP
- Publication
- Experiments
- Investigation
- Study
- Assay
- Activities
- Presentation
- Event
- Admin
- Programme
- Project
- Institution
- Profile

Project centric approach

[Home](#) > [Projects Index](#) > MOSES

MOSES (Micro Organism Systems biology: Energy and *Saccharomyces cerevisiae*) develops a new Systems Biology approach, which is called 'domino systems biology'. It uses this to unravel the role of cellular free energy ('ATP') in the control and regulation of cell function. MOSES operates through continuous iterations between partner groups through a new systems-biology driven data-management workflow. MOSES also tries to serve as a substrate for three or more other SYSMO programs.



Programme: SysMO

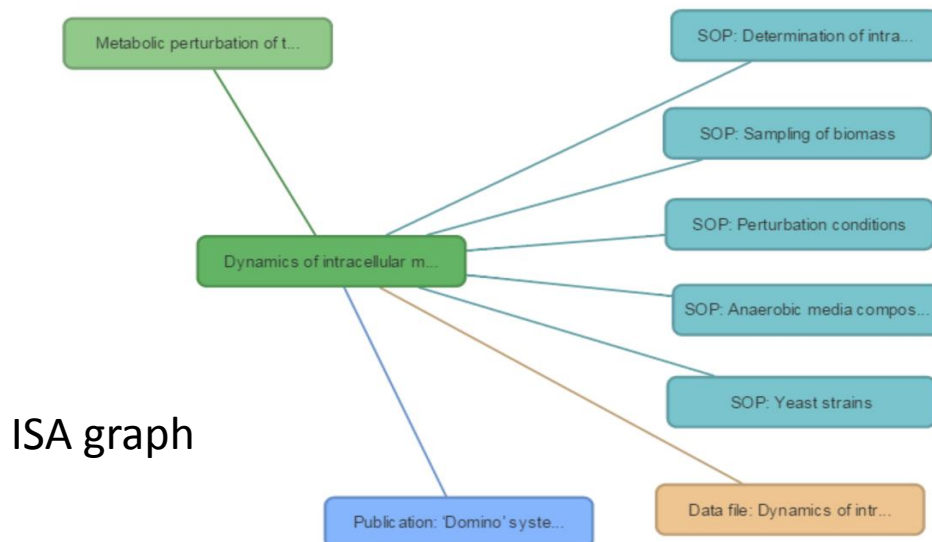
Public web page: <http://www.moses.sys-bio.net/>

Organisms: *Saccharomyces cerevisiae*

FAIRDOM PALs: Femke Mensonides, Maksim Zakhartsev, Walter Glaser

Related items

[People \(20\)](#)
[Institutions \(6\)](#)
[Investigations \(3\)](#)
[Studies \(8\)](#)
[Assays \(12+1\)](#)
[Samples \(0+4\)](#)
[Cell cultures \(0+4\)](#)
[Strains \(1\)](#)
[Data files \(9+1\)](#)
[Models \(1+2\)](#)
[SOPs \(7+4\)](#)
[Publications \(5\)](#)

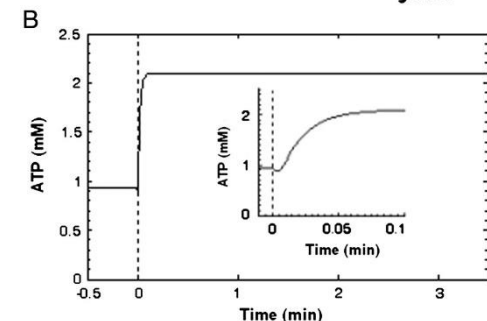
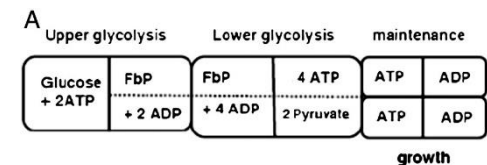


Experimental

Assay: Dynamics of intracellular metabolites during glucose pulse

Connected items

Data file: Dynamics of intracellular metabolites during glucose pulse
SOP: Yeast strains
SOP: Anaerobic media composition
SOP: Perturbation conditions
SOP: Sampling of biomass



[Home](#) / [Projects Index](#) / [EmPowerPutida](#)



EmPowerPutida

Asset report

Administration ▾

Exploiting native endowments by re-factoring, re-programming and implementing novel control loops in *Pseudomonas putida* for bespoke biocatalysis. The EmPowerPutida project aims to engineer the lifestyle of *Pseudomonas putida* to generate a tailored, re-factored chassis for the production of so far non-accessible biological compounds. *Pseudomonas putida* is a bacterium with a highly versatile metabolism, including the capability to degrade or produce organic chemicals.



Programme: [Independent Projects](#)

Public web page: <http://www.empowerputida.eu/>

Internal web page: *Not specified*

Organisms: [Pseudomonas putida](#)

FAIRDOM PALs: *No PALs for this Project*

Storage Usage

The total size of all project assets is: **0 Bytes**

Related items

People (16)

Institutions (9)

[Ruben Van Heck](#)



Projects: [EmPowerPutida](#)
Institutions: [University of Wageningen](#)
Email: rubenvanheck@gmail.com
Web page: *Not specified*
Phone: *Not specified*
Skype: *Not specified*

Disciplines: *Not specified*
Roles: *Not specified*
Expertise: *Not specified*
Tools: *Not specified*

[Victor De Lorenzo](#)



Projects: [PSYSMO](#), [EmPowerPutida](#)
Institutions: [CSIC Madrid](#), [CSIC](#)
Email: vdlorenzo@cnb.csic.es
Web page: *Not specified*
Phone: *Not specified*
Skype: *Not specified*

Disciplines: *Not specified*
Roles: *Not specified*
Expertise: *Not specified*
Tools: *Not specified*

Data file - Register vs. Upload



FAIRDOM



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Search



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New Data file

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Local file

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File to upload *

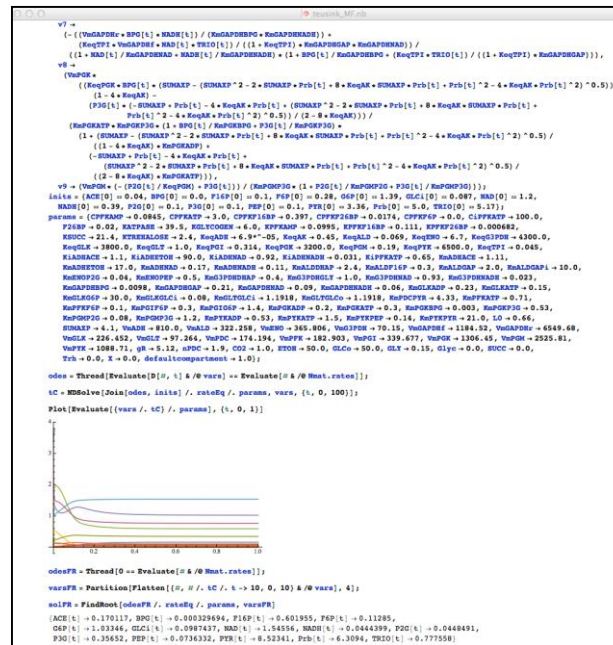
Datei auswählen

Wegbeschre..._Engl.doc

Choose if to register or
upload

The data contained within the files can be very ambiguous.

C14		
	A	B
1	A steady state with given resolution was found.	
2		
3	Species	Concentration (mmol/l)
4	Extracellular Glucose	50
5	Glucose in Cytosol	0.0987587
6	Glucose 6 Phosphate	1.03325
7	Fructose 6 Phosphate	0.112813
8	Fructose-1,6 bisphosphate	0.601908
9	Triose-phosphate	0.777524
10	1,3-bisphosphoglycerate	0.000329574
11	3-phosphoglycerate	0.356484
12	2-phosphoglycerate	0.0448437
13	Phosphoenolpyruvate	0.0736168
14	Pyruvate	8.52315
15	Acetaldehyde	0.170114
16	High energy phosphates	6.30888
17	NAD	1.54556
18	NADH	0.0444402



C14		
	A	B
31	Reaction	Flux (mmol/min)
32	Hexokinase	88.1495
33	Glucose-6-phosphate isomerase	77.3495
34	Glycogen synthesis	6
35	Trehalose 6-phosphate synthase	2.4
36	Phosphofructokinase	77.3495
37	Aldolase	77.3495
38	Glyceraldehyde 3-phosphate dehydrogenase	136.497
39	Phosphoglycerate kinase	136.497
40	Phosphoglycerate mutase	136.497
41	Enolase	136.497
42	Pyruvate kinase	136.497
43	Pyruvate decarboxylase	136.497
44	Succinate synthesis	3.64045
45	Glucose transport	88.1495
46	Alcohol dehydrogenase	129.216
47	Glycerol 3-phosphate dehydrogenase	18.2022
48	ATPase activity	84.5328

Standardisation helps understanding and exchange



Capture & Curate Data: Spreadsheet tools

Element	Investigation Title	Format	Constraint	Type	Key Type	Explanations
1	Example	Text	Not NULL		PK	
2	Transcription profiling of wild-type and ATF3	Text	Not NULL		CV	
3						
4						
5	Experimental Design Type *	Text	Not NULL		PK	Explanations
6	Experimental Factor Category *	Text	Not NULL		CV	PK - primary key
7	Person Last Name	Text	Not NULL		CV	PK - foreign key
8	Person First Name	Text	Not NULL		CV	CV - controlled vocabularies
9	Person Mid Initial	Text	Not NULL			
10	Person Affiliation	Text	Not NULL			
11	Roles *	Text	Not NULL			
12	Quality Control Description Type *	Text	Not NULL		CV	
13	Replicate Description Type *	Text	Not NULL		CV	
14	Normalization Description type *	Text	Not NULL		CV	
15					CV	
16	Experiment Description	Text	Not NULL		CV	
17	Protocol Name	Text	Not NULL		CV	
18	Protocol Type *	Text	Not NULL		CV	
19	Protocol Description	Text	Not NULL		CV	
20	Protocol Parameters	Text	Not NULL		CV	
21	SDRF File	Text	Not NULL		CV	
22	data file	Text	Not NULL		CV	
23	ADF file	Text	Not NULL		CV	
24	Term Source Name	Text	Not NULL		CV	
25	Term Source File	Text	Not NULL		CV	
26	Term Source Version	Text	Not NULL		CV	
27					CV	
28					CV	
29					CV	
30					CV	
31					CV	
32					CV	
33					CV	
34					CV	
35					CV	
36					CV	
37					CV	
38					CV	
39					CV	
40					CV	
41					CV	
42					CV	
43					CV	
44					CV	
45					CV	

- Admins create spreadsheet with ontology-annotated selection lists
- Users helped in providing annotated data

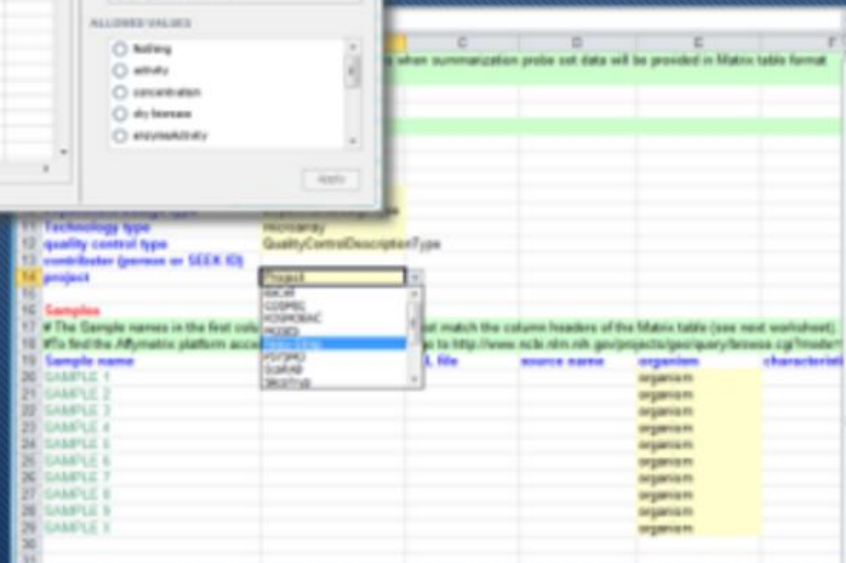
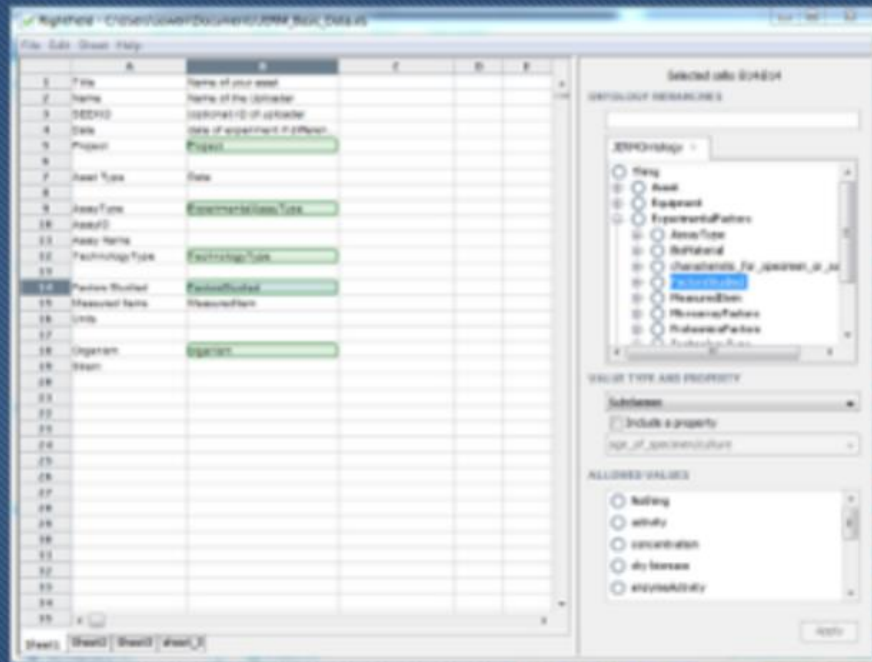
Instrument Excel template sheets to annotate with **controlled vocabulary terms**

Self-contained data package

Upload, index, discover, process, compare in SEEK

<http://www.rightfield.org.uk>

Biosamples can be defined according to Minimum Information Models either directly in SEEK (with output of Rightfield annotated spreadsheet), or Through input of Rightfield annotated spreadsheets.





Chip-chip Excel data



Unsubscribe



View samples



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Explore

	Metadata Template	Matrix	Metadata Example	Samples	Matrix Example					
	A	B	C	D	E	F	G	H	I	
1	Sample name	title	raw data file 1	raw data file 2	ch1: source name	ch1: organism	ch1: ch1	ch1: ch1	ch1	
2	Sample 1	RAG H3K4me2	RAG_H3K4me2_Cy5.pair	RAG_H3K4me2_Cy3.pair	H3K4me2 ChIP DNA from Rag2-/- pro-B cells	Mus musculus	Rag2-/-	pro-B cell	C5	
3	Sample 2	RAG H3K4me3	RAG_H3K4me3_Cy5.pair	RAG_H3K4me3_Cy3.pair	H3K4me3 ChIP DNA from H3K9ac ChIP DNA from Rag2-/- pro-B cells	Mus musculus	Rag2-/-	pro-B cell	C5	
4	Sample 3	RAG H3K9ac	RAG_H3K9ac_Cy5.pair	RAG_H3K9ac_Cy3.pair	H3K9ac ChIP DNA from Pax5-/- Rag2-/- pro-B cells	Mus musculus	Pax5-/-	pro-B cell	C5	
5	Sample 4	P5R2 H3K4me3	P5R2_H3K4me3_Cy5.pair	P5R2_H3K4me3_Cy3.pair	H3K4me3 ChIP DNA from Pax5-/- Rag2-/- pro-B cell	Mus musculus	Pax5-/-	pro-B cell	C5	
6	Sample 5	P5R2 H3K4me2	P5R2_H3K4me2_Cy5.pair	P5R2_H3K4me2_Cy3.pair	H3K4me2 ChIP DNA from Pax5-/- Rag2-/- pro-B cell	Mus musculus	Pax5-/-	pro-B cell	C5	
7	Sample 6	RAG H3K9ac	RAG_H3K9ac_Cy5.pair	RAG_H3K9ac_Cy3.pair	H3K9ac ChIP DNA from Rag2-/- pro-B cells	Mus musculus	Rag2-/-	pro-B cell	C5	
8										

Samples

Show 5 entries

Sample name	title	raw data file 1	raw data file 2	ch1: source name	ch1: organism
Sample 1	RAG H3K4me2	RAG_H3K4me2_Cy5.pair	RAG_H3K4me2_Cy3.pair	H3K4me2 ChIP DNA from Rag2-/- pro-B cells	Mus musculus
Sample 2	RAG H3K4me3	RAG_H3K4me3_Cy5.pair	RAG_H3K4me3_Cy3.pair	H3K4me3 ChIP DNA from H3K9ac ChIP DNA from Rag2-/- pro-B cells	Mus musculus
Sample 3	RAG H3K9ac	RAG_H3K9ac_Cy5.pair	RAG_H3K9ac_Cy3.pair	H3K9ac ChIP DNA from Pax5-/- pro-B cells	Mus musculus
Sample 6	RAG H3K9ac	RAG_H3K9ac_Cy5.pair	RAG_H3K9ac_Cy3.pair	H3K9ac ChIP DNA from Rag2-/- pro-B cells	Mus musculus



Sample 1

Sample type: Chip-chip Excel

Source data: Chip-chip Excel data

Sample name: Sample 1

title: RAG H3K4me2

raw data file 1: RAG_H3K4me2_Cy5.pair

raw data file 2: RAG_H3K4me2_Cy3.pair

ch1: source name: H3K4me2 ChIP DNA from Rag2-/- pro-B cells

ch1: organism: Mus musculus

ch1: characteristics: Genotype: Rag2-/-

ch1: characteristics: Cell type: pro-B cells

ch1: characteristics: Strain: C57BL/6J

ch1: characteristics: ChIP Antibody: H3K4me2

ch1: molecule: genomic DNA

ch1: label: Cy5

ch1: treatment protocol: Rag2-/- pro-B cells were MACs sorted from the bone

Related items

People (1)

Investigations (1)

Studies (1)

Assays (1)

Data files (1)

Chip-chip Excel

No description specified

Template

GA_CHIP_chip_w_platt SEEKJERM_edited.xls - Download

Attributes

- Sample name (String) *
- title (String) *
- raw data file 1 (String) *
- raw data file 2 (String) *
- ch1: source name (String) *
- ch1: organism (String) *
- ch1: characteristics: Genotype (String) *
- ch1: characteristics: Cell type (String) *
- ch1: characteristics: Strain (String) *
- ch1: characteristics: ChIP Antibody (String) *
- ch1: molecule (String) *
- ch1: label (String) *
- ch1: treatment protocol (String) *
- ch1: growth protocol (String) *
- ch2: source name (String) *
- ch2: organism (String) *
- ch2: characteristics: Genotype (String) *
- ch2: characteristics: Cell type (String) *
- ch2: characteristics: Strain (String) *
- ch2: characteristics: ChIP Antibody (String) *
- ch2: molecule (String) *
- ch2: label (String) *
- ch2: treatment protocol (String) *

Biosample instance
(type based)

Biosample
type

Standard Operating Procedures

[Home](#) > [SOPs Index](#) > Introduction of shRNAs, miRNAs or anti-microRNAs into primary human hepatocytes with lentivirus



Introduction of shRNAs, miRNAs or anti-microRNAs into primary human hepatocytes with lentivirus



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View content

Here we used VSV-G-pseudotyped, EGFP-expressing lentiviral vectors to develop an efficient gene transfer protocol to modify gene expression in primary human hepatocytes (by RNAi). The protocol comprises the production of recombinant viruses as well as the steps for efficient delivery of short-hairpin RNA (shRNAs), microRNAs or anti-microRNAs to human hepatocytes. On average infection efficiencies of over 95% are achieved at relatively low multiplicity of infection (MOI), which effectively reduces the amount of preparative work required per experiment. Depending on the laboratory equipment available, we provide here two alternative workflows, which can be easily adapted in the lab. The procedure of virus production with subsequent titer determination takes approx. 6 to 10 working days. The procedure of viral infection of hepatocytes until effects can be measured takes approx. 3 to 5 days. This protocol should be helpful to study many aspects of functional genomics in primary human hepatocytes.

Contributors

[Maria Thomas]

Attributions

None

Scales

Not Specified

Filename: Lentiviral production and infection_SOP_04042011.pdf

Format: PDF document

MATERIALS

REAGENTS/KITS

BLOCK-iT™ Lentiviral RNAi Expression Kit (Invitrogen#49-4400)

ViraPower™ Lentiviral Gateway Expression Kit (Invitrogen#K49-6000)

miRZip™ Lentivector-based Anti- MicroRNAs (System Biosciences#MZIPxxxPA/AA-1)

miRZip™ Lentivector-based Anti- microRNAs (System Biosciences#PMIRHxxxPA/AA-1)

PROCEDURE

NOTE: all the steps marked with "S" should be performed following recommended guidelines for working with BL-2 organisms (Germany: S2 lab).

1. Preparation of HEK293FT cells.

For cultivating HEK293FT cells, add G148 (Geneticin, final concentration 500 µg/ml) to the DMEM culture medium with components (see Reagent Setup). The cells should be passaged at least 1-2 times after thawing to adapt to the culture conditions. Three days prior to transfection, plate out the cells at a density of approximately 3.5×10^5 cells/per 1 T175 flask in 30 ml of medium with components and G148 to achieve optimal phase of cellular growth.

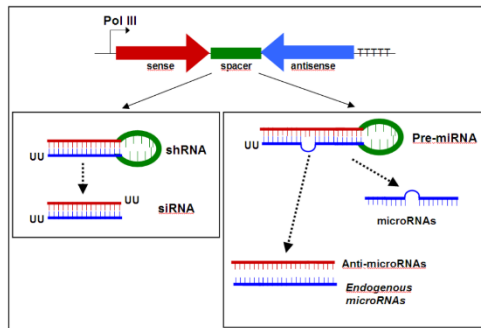


Fig.1: Schematic presentation of designed template sequences which are processed intracellularly into short hairpin RNAs, microRNAs or anti-microRNAs. The stem-loop structures consisting of both the sense and anti-sense strands of the targeted sequence are separated by a loop sequence.

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Step 1 → Step 2 → Step 3

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Carole Goble |

no access

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Just Enough Sharing

Access
Permissions

Also include people in my..

- ☐ - "white list", who always get full access [\[create \]](#)
- ☐ - "black list", who have no access at all [\[create \]](#)

and research

[Home](#) / [Models Index](#) / Kinetic model for incubation (penkler2)

Kinetic model for incubation (penkler2) Version 7 ▾

[⚡ Simulate Model on JWS](#)[👁 Find related Data files](#)[📧 Subscribe](#)[📄 Download](#)

Glycolytic model for Plasmodium

system

3 items are associated with this model

[🖼 Image icon](#)

Filename	Format
penkler2.xml	XML document
penkler2.nb	Mathematica notebook
penkler2.dat	unencoded

Version 7 (latest)

Version 6

Version 5

Version 4

Version 3

Version 2

Version 1 (earliest)

Organism: *Not specified***Model type:** Ordinary differential equations**Model format:** SBML**Execution or visualisation environment:** JWS Online**Model image:** *No image specified*[👤 Contributors](#)[Activity](#)**Views:** 258 **Downloads:** 31

Created: 11th Aug 2014 at 09:58

Last updated: 1st Jul 2015 at 10:19

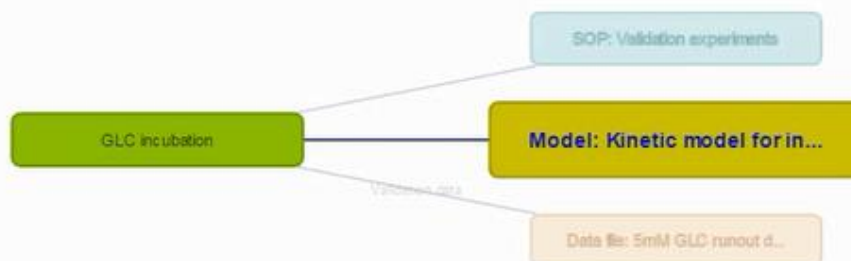
Last used: 10th Jul 2015 at 15:53

[🏷 Tags](#)

plasmodium

[🔄 Update your tags ▾](#)[👤 Attributions](#)

None

Selected item: **Model:** Kinetic model for incubation (penkler2)

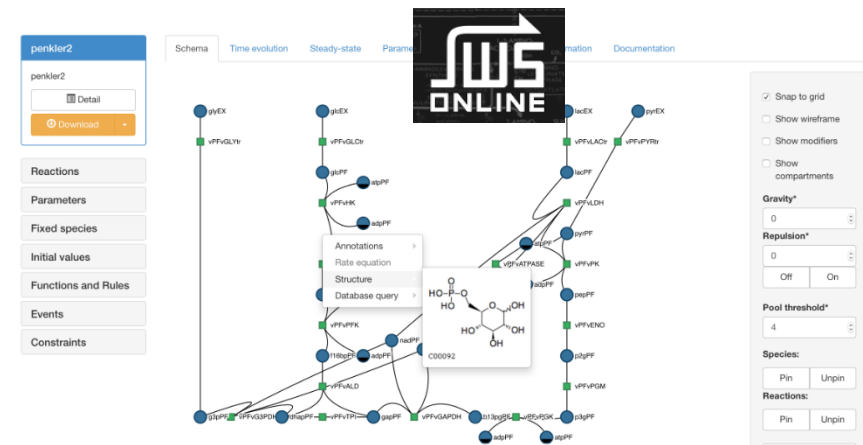
Double-click to go to fullscreen,

Middle-ollok:
 pin/unpin nodes
 Shift-ollok:
 pool/unpool species
 Right-ollok: context
 menu

... with integrated tooling

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

SBML Model simulation



Deletions are coloured in red and insertions are coloured in blue

SBML Differences

Both documents have same Level/Version: L3V1

Model versioning

Parameters

VappSPSSPP Attribute *value* has changed: 797 → 500

Compartments

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

Species

Sucrose	Attribute <i>compartment</i> has changed: default_compartment → main
ADPGam	Attribute <i>compartment</i> has changed: default_compartment → main
PPam	Attribute <i>compartment</i> has changed: default_compartment → main
Pcvt	Attribute <i>compartment</i> has changed: default_compartment → main
F6Pcvt	Attribute <i>compartment</i> has changed: default_compartment → main
ADPam	Attribute <i>compartment</i> has changed: default_compartment → main
UDPcvt	Attribute <i>compartment</i> has changed: default_compartment → main
Glucoseam	Attribute <i>compartment</i> has changed: default_compartment → main
G6Pam	Attribute <i>compartment</i> has changed: default_compartment → main

Reproducing simulations

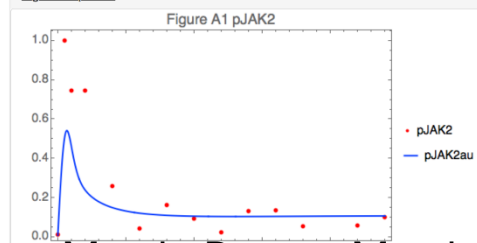
JWS Online Model Database - Simulation

SED-ML Simulation Result: bachmann2011

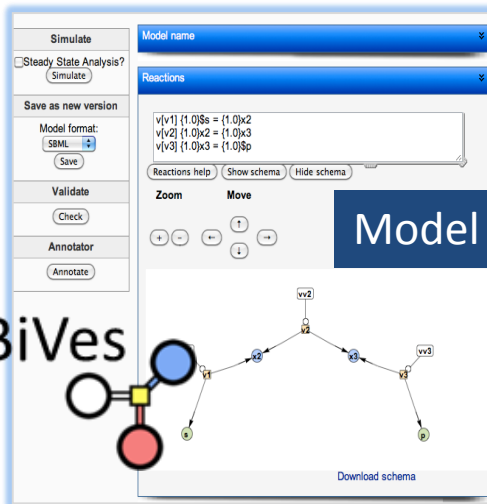
Details Download Create derivative

powered by
SEMS FAIRDOM

Figure A1 pJAK2



Model comparison



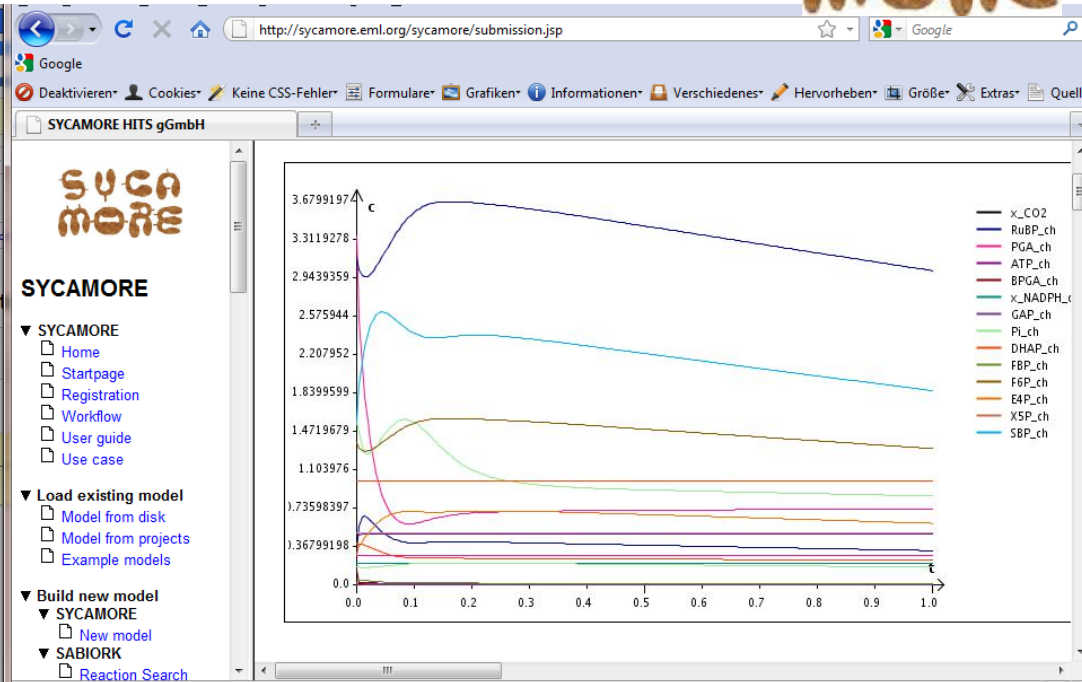
[Jacky Snoep, Dagmar Waltemate, Martin Peters, Martin Scharm]

Integration of Modelling Platforms

Models in SEEK can be directly transferred to and subsequently edited, processed and simulated in JWS online, SYCAMORE or Cytoscape Web

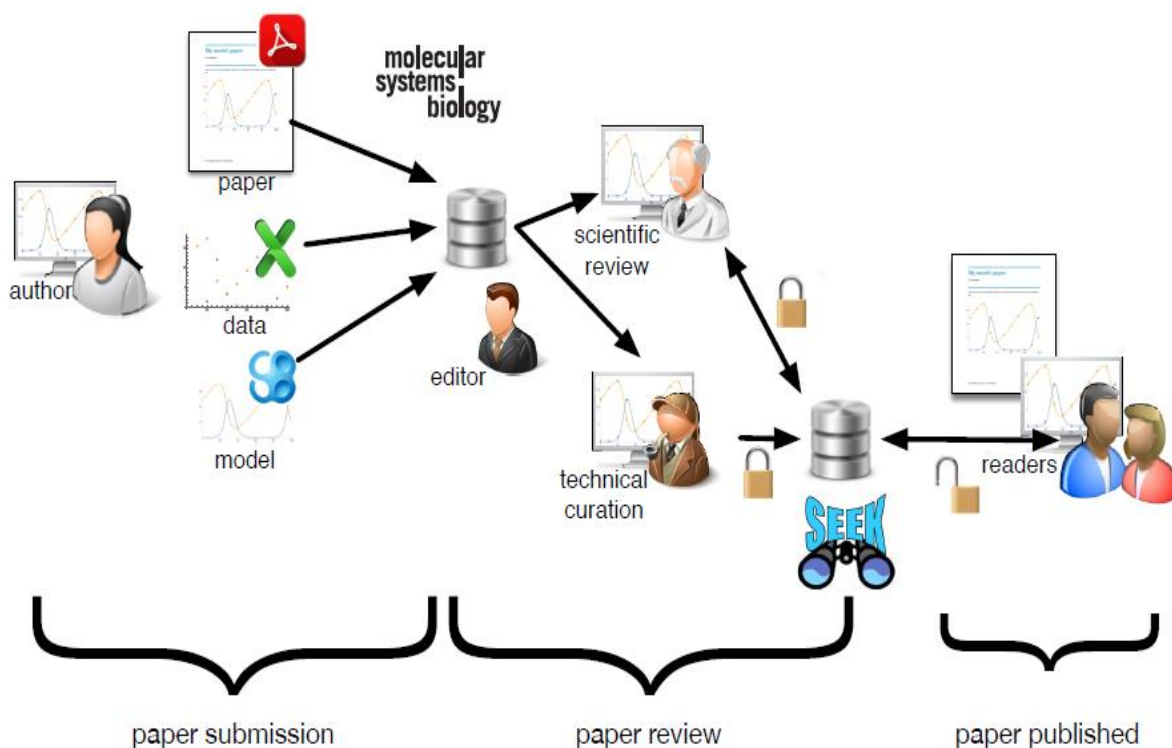


This screenshot shows the SYCAMORE web interface. At the top, there are navigation tabs: "Yellow Pages", "ISA", "Assets", "Forums", and "Events". Below these is a "Provide Feedback" section. The main content area displays a yellow message: "Model was successfully uploaded and saved." Below this message are buttons for "Unsubscribe", "Upload new version", "Manage Model", and "Download Model". There are also buttons for "JWS One Stop" and "Simulate Model". A status message says "This item is Shared, but not with all visitors". Below this, the model details for "Biomodels 13" are shown, including the title, file name (BIOMD0000000013.xml), format (XML document), organism (Not specified), model type (Not specified), and model format (Not specified). The version is "Version 1 (of 1)" and was created on 26/08/2011 at 08:53:28 by David Shockley. On the left side, there is a sidebar with "Announcements" and "Favourites" sections. The "Tags" section lists various biological and computational terms.



Reproducible model simulations in papers using SED-ML

Publishing reproducible model simulations



Three tiered service

- + store DOI citable supplementary files on FAIRDOMHub
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- +++ reproducible clickable figures in papers using SED-ML

[Jacky Snoep, Dagmar Waltemath]

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Register Publication

Choose whether to search by PubMed ID or DOI using the dropdown menu below, then enter the document identifier into the text box and click "Fetch".
If SEEK successfully retrieves your publication, click "Register" to process to the next step.

PubMed ID ▾

Please select the Projects this publication is related to. You must select a Project, and it must be a Project you are a member of.

 Projects ▾

The following projects are associated with this publication:

None

Create snapshot and get DOI for your research asset

Snapshot 8 (25th Apr 2016) 

DOI: 10.15490/seek.1.investigation.74

<https://fairdomhub.org/investigations/74/snapshots/8>

DOI: [10.15490/seek.1.investigation.74.8](https://doi.org/10.15490/seek.1.investigation.74.8)

Created at: 25th Apr 2016 at 07:32

Investigation: Metabolic analysis
of effects of sucrose translocation
on phenotypic traits of
Arabidopsis t...

Study: Analysis of central carbon
and energy metabolisms of
growing Arabidopsis thaliana in
relation to suc...

Model: ZucAt: multi-compartment
metabolic model of growing
Arabidopsis thaliana

Modelling Analysis: Flux Balance
Analysis of multi-compartment
metabolic model of growing
Arabidopsis thaliana

Data file: ZucAt: FBA solution of
the model under dark growth
conditions

Data file: ZucAt: The
stoichiometric matrix of the model

Data file: ZucAt: The compound
database

Data file: ZucAt: The gene
database

Data file: ZucAt: The transformers
database

Data file: ZucAt: FBA solution of
the model under light growth
conditions (I)

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

Gerald Penkler^{1,2}, Francois du Toit¹, Waldo Adams¹, Marina Rautenbach¹, Daniel C. Palm¹, David D. van Niekerk¹ 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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Tel: +27 (0)2180 85844
E-mail: jls@sun.ac.za

(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://ijb.bio.vu.nl/database/penkler>). The investigation and complete experimental data set is available on SEEK (10.15490/seek.1.investigation.56).

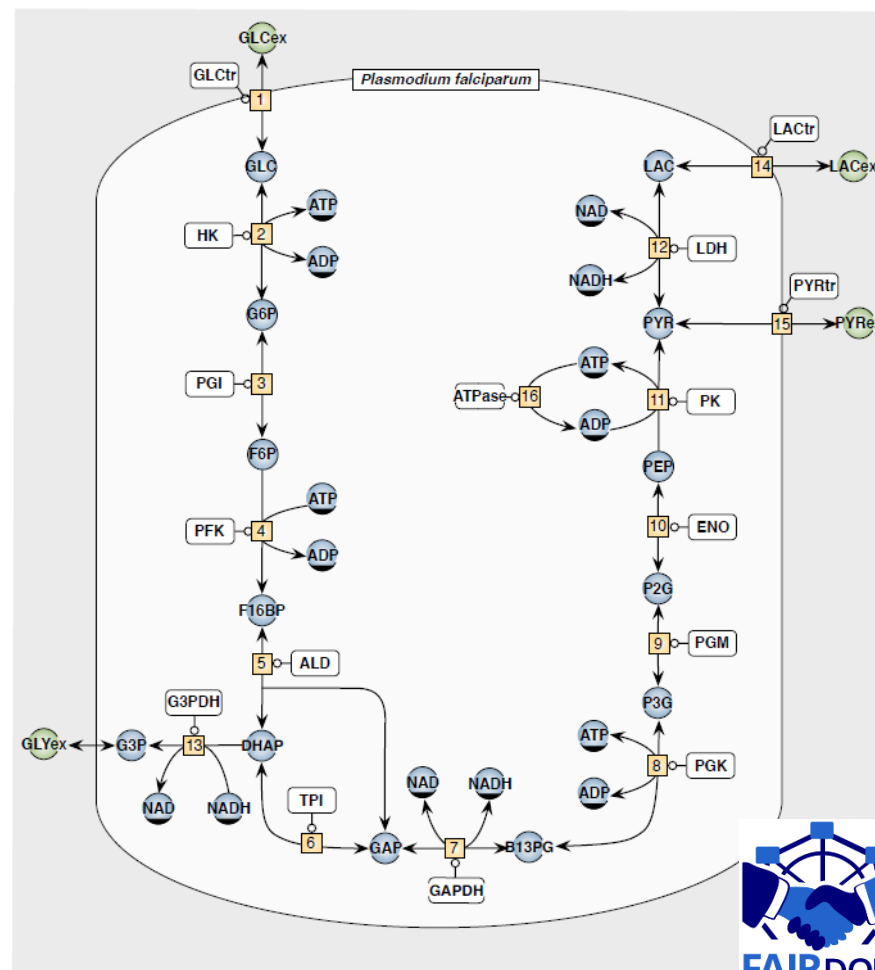
Introduction

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, and subsequent

Abbreviations

2PG, 2-phosphoglycerate; 3PG, 3-phosphoglycerate; ALD, fructose-bisphosphate aldolase; B13PG, 1,3-bisphosphoglycerate; DHAP, glyceraldehyde 3-phosphate; ENO, phosphoenolpyruvate hydratase; F16BP, fructose 1,6-bisphosphate; F6P, fructose 6-phosphate; G3P, glyceraldehyde 3-phosphate; G3PDH, glyceraldehyde 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.



Example: Virtual Liver SEEK

Virtual Liver SEEK x

seek.virtual-liver.de

SEEK

virtual liver network

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Fluidigm HepatoSys IL-6
inflammation Insulin signalling Kinetic
Modelling logical modelling LPS LPS
showcase metabolism
MidtermReview Nuclear receptors
ODE primary human hepatocytes
Report systemic iron homeostasis
TNFalpha VLN

Organisms

Homo sapiens
Mus musculus

Browse by Scale

All -
Organism -
Liver -
Liver lobule -
Intercellular -
Cell -

+

Investigations (93) Studies (56) Assays (85) Samples (250) Specimens (248) Strains (14) Data files (1636) Models (129) SOPs (58) Publications (448) Presentations (639) Events (137)

Integration of intracellular ODE models

ID: 6

Studies: Integration of intracellular signaling pathways

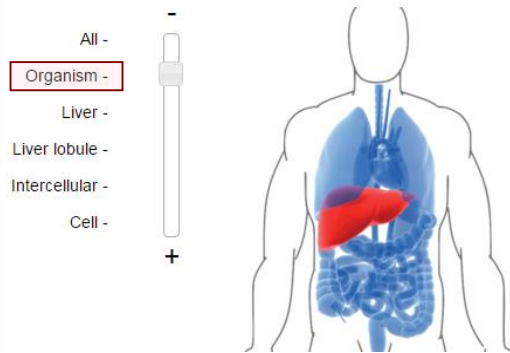
Scales: Cell

No description specified

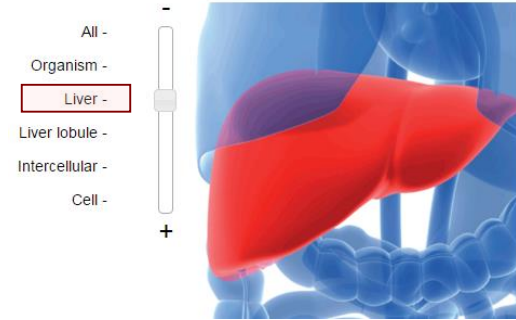
Projects: E1: Integration on the cellular level

Virtual Liver Data - browse by scale

Browse by Scale



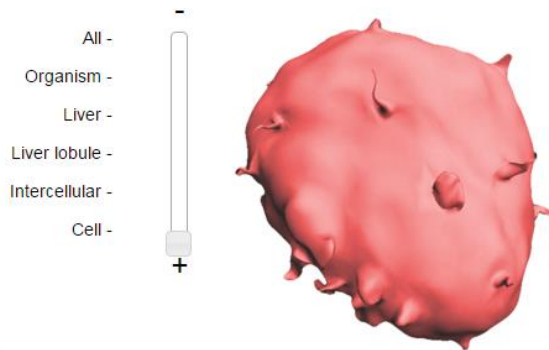
Browse by Scale



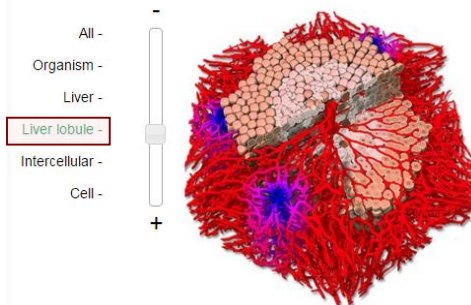
Investigations (8) Studies (12) Assays (14) Samples (19) Specimens (10) Data files (97) Models (8) SOPs (11) Publications (56) Presentations (99)

Investigations (3) Studies (1) Specimens (26) Data files (19) Models (9) SOPs (7) Publications (28) Presentations (64)

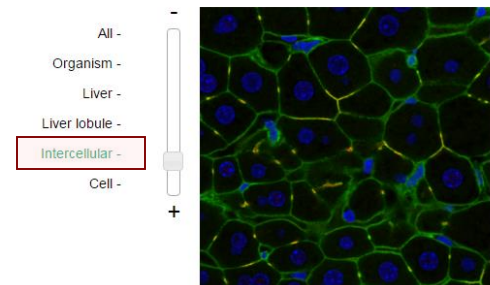
Browse by Scale



Browse by Scale



Browse by Scale



Investigations (25) Studies (35) Assays (45) Samples (32) Specimens (16) Data files (284) Models (86) SOPs (26) Publications (158) Presentations (210)

SEEK for NMTrypl



Ulrike Wittig



New Medicines
for Trypanosomatidic Infections

HOME

About NMTrypl

PARTNERS

NEWS & EVENTS

FP7 Projects

CONTACT

NEWS

- > Drug Development for Neglected Parasitic Diseases Funded projects, Modena, June 2016

Location: UNIMORE, Modena, Italy

Start day: 15-06-16

End Day: 16-06-16

For more information please click here

1 2

PRESS & PUBLICATIONS

- > NMTrypl communication and dissemination activities

The complete list of communication and dissemination activities of NMTrypl project is available [here](#). For additional information, please visit the "news and events" session.

NMTRYPI PROJECT



ABSTRACT

The **NMTrypl concept** is based on the development of **innovative drug leads** including a mechanism-based combination of a known and investigational drug and dual targets inhibition by using a **common drug discovery platform**. The platform is established by experts in their respective fields from SMEs and the public research sector in Europe and in disease-endemic countries.

The innovative concept is reinforced by the identification of preclinical **biomarkers** enabling the proteomic profiling of the compound to understand the mechanism of action (MoA biomarker) and to detect the efficacy of the lead candidate (pharmacodynamic biomarkers).

The new NMTrypl platform will perform the screening of compound libraries, lead development, testing in mice, hamsters and dogs as a reservoir of the visceral leishmaniasis disease as well as **toxicology** and **safety testing** (*in vitro* against cellular types and *in vivo* in animals) to overcome current limitations in

Automatic detection of protein IDs and link to UniprotKB and StringDB



Find, share and exchange **Data**, **Models** and **Processes** within the NMTryp Project.

Yellow pages | Experiments | Assets | Activities | Documentation

Data files | SOPs | Publications

Search here...

New or upload

CREATE

Go to my Project

My Project

Announcements

NMTryp SEEK members are assigned to all work packages about 1 month ago by Ulrike Wittig

Favourites

Tags [show all]

computational structural biology
molecular modeling PTR1
Summarized Data
Tbrucei

Organisms

Canis lupus familiaris
Cricetulus griseus
Leishmania donovani
Leishmania infantum

Home > Data files Index > proteins_uniprotID_example > Explore

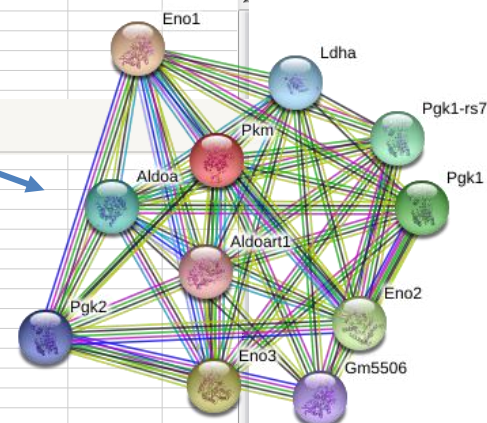
D2 P52480

List Annotations | Add Annotation | Export Data | Plot Data | Clear Selection | Heat Map | Parallel Coordinates

Sheet1 | Sheet2 | Sheet3

	A	B	C	D	E	F	G	H	I	J
1	protein name	organism	tissue	UniprotID						
2	Pyruvate kinase	Mus musculus	muscle	P52480						
3	Pyruvate kinase	Homo sapiens	liver	P30111	Link to UniProt					
4	Pyruvate kinase	Rattus norvegicus	muscle	P11307	Link to String DB					
5	Hexokinase-1	Homo sapiens	brain	P19307						
6	Hexokinase-2	Homo sapiens	muscle	P52789						
7										
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16										
17										
18										
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20										
21										
22										

STRING



UniProtKB

BLAST | Align | Retrieve/ID mapping

UniProtKB - P52480 (KP YM_MOUSE)

Display

BLAST | Align | Format | Add to basket | History

Entry

Feature viewer

Feature table

None

Function

Names & Taxonomy

Subcell. location

Protein | Pyruvate kinase PKM

Gene | Pkm

Organism | Mus musculus (Mouse)

Status | Reviewed - Annotation score: 5 - Experiment

Function

Glycolytic enzyme that catalyzes the transfer of a phosphoryl group from

Legend | Data Settings | View Settings | Tables / Exports | Evidence | Analysis



Experiments

Copurification, co-crystallization, Yeast2Hybrid, Genetic Interactions, etc ... as imported from primary sources.



Databases

Known metabolic pathways, protein complexes, signal transduction pathways, etc ... from curated databases.



Neighborhood

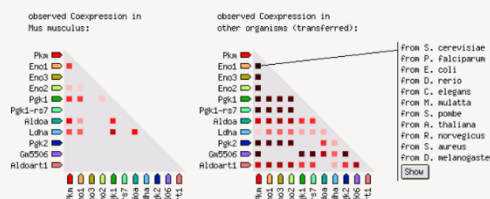
Groups of genes that are frequently observed in each other's genomic neighborhood.



Cooccurrence

Gene families whose occurrence patterns across genomes show similarities.

GENE COEXPRESSION



New Medicines for
Trypanosomatid Infections

Visualization of enzyme inhibition by different compounds (in %)

Heat map + Parallel coordinates plot



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Tags [show all]

computational structural molecular modeling F

Summarized D

Tbrucei

Organisms

Canis lupus familiaris

Cricetus griseus

Leishmania donovani

Leishmania infantum

Leishmania major

Home > Data files Index > Tranche1_Nov2014 > Explore

XXXXXX Avg % Inhibition, hERG

List Annotations Add Annotation Export Data Plot Data Clear Selection Heat Map Parallel Coordinates

Data heatmap Close

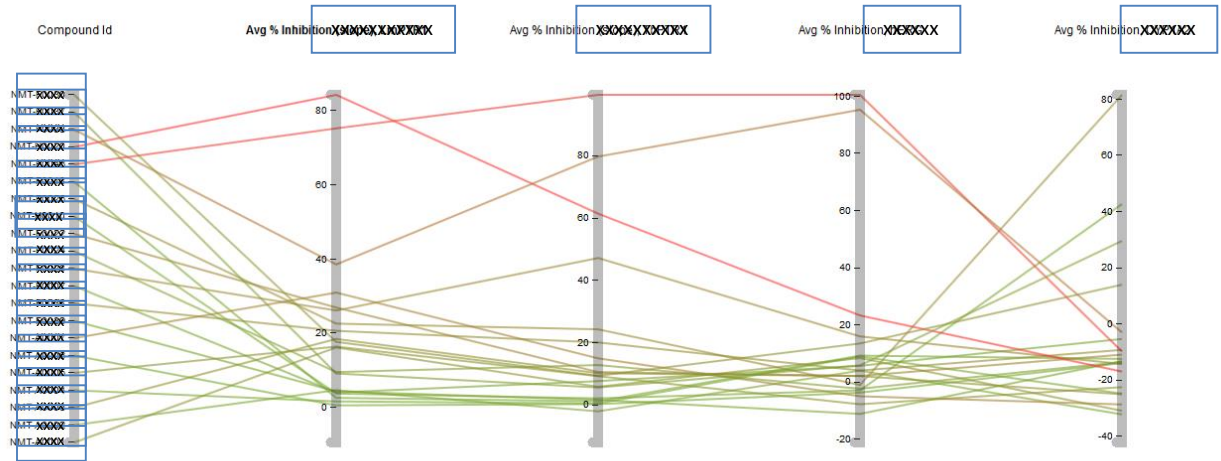
+ -- Save as SVG

Screening (slider change): -453,-13.5,27.8,103



J	K	L	M	N	O	P	Q	R	S
0	4.100000	5.326956	no	10	-9.143333	11.89742	10	-19.15666	1.232
0	5.739999	3.900230	no	10	-5.263333	10.18506	10	-7.993333	0.846
0	16.02666	6.331784	no	10	-14.18	7.055810	10	21.87333	4.306
0	-2.276666	10.24087	no	10	-13.43	12.31797	10	-30.57333	6.770
0	2.213333	8.356810	no	10	-10.83	9.717297	10	-22.02333	3.958
0	-2.826666	5.805137	no	10	42.74666	3.331189	10	-220.153	7.184
0	-0.950000	5.361367	no	10	81.62666	3.561220	10	72.50333	2.593
0	9.32	9.142913	no	10	-12.36	6.099743	10	-13.76333	3.416
0	100.55	7.899902	no	10	-9.74	4.961538	10	47.77	32.47
0	23.36	9.398024	no	10	-16.87666	3.315673	10	10.82999	5.629
0	95.35000	7.994452	no	10	-2.946666	3.354900	10	-3.096666	4.800
0	5.906666	7.064282	no	10	29.64666	2.851401	10	-19.76666	1.703

Parallel Coordinates Plot Close



Brush mode: 1D-axes Predicate: AND Reset Brushes Export PNG





We help to build/judge
DMM plans

Data management checklist

ERASysAPP DMMcore checklist document

The goal of this checklist is to help facilitate the planning and writing of the Data and Model Management part of an ERASysAPP proposal.

For any questions, please contact ptj-dmmcore@fz-juelich.de or participate in the DMMcore webinars ([go to registration for webinars](#)).

There will be a centrally funded DMMCore project which plans to offer the following facilities to all projects:

Data management

- Management facilities for project data
- Secure and private storage and management of your data
- First-class management of spreadsheet data
- Permanent storage and management of large scale data up to 1.5TB/Project (for dedicated storage of data beyond 1.5TB/Project, please contact ptj-dmmcore@fz-juelich.de. The data is kept 10 years beyond the project lifetime.

Metadata management

- Linking to data stored at outside resources
- Interlinking and management of SOPs, data, models, people, projects, publications
- Cataloguing and metadata management of data, models and SOPs
- Support with use of standards and vocabularies.

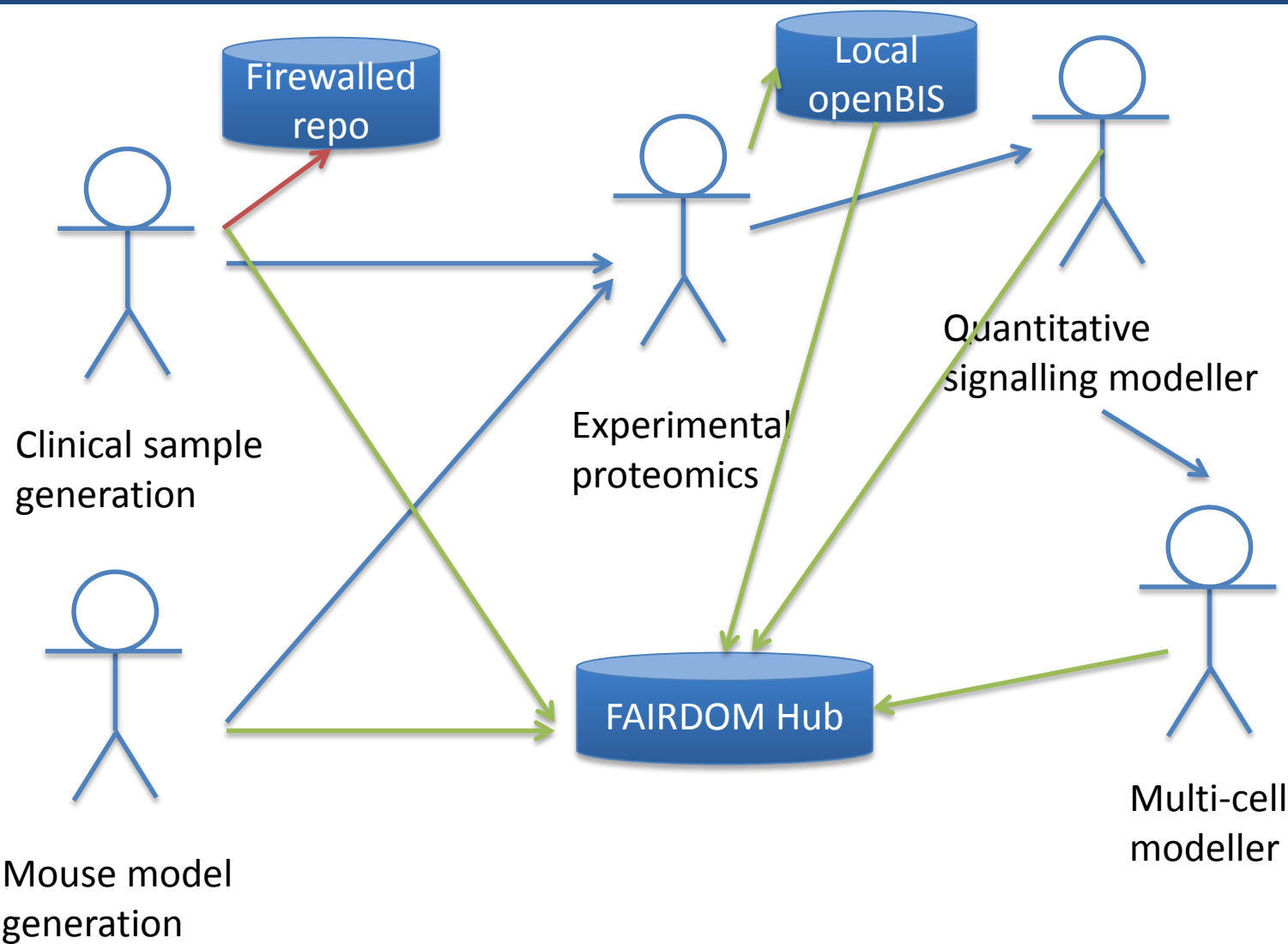
Question support

DMM checklist

Questions about

- Amount of Data/Model/SOP **storage**
- About data **flows**
- About **Meta** data needs
- About **sequence** of needs
- About people responsible (contacts) for DMM
- Needs judges with experience

Example: How is the data flow?





Tiers of possible
support

Three tiers of possible support

- **Best effort** tier:
 - Feasible with current resources
 - In completely line with our remit
 - No specific support
- **Subcontract** tier: Requires Subcontract
 - Close to our remit
 - Not feasible with our current resources
 - Short-term/punctual
- **Partnership** tier: Requires Partnership
 - Not feasible with our current resources
 - Long-term/continuous

Increasing adoption

Increasing quality

Increasing involvement



Tiers software platform

Tier	Proposed
Best effort	<ul style="list-style-type: none">• Get and install software from GitHub repository• Use FAIRDOM Hub• Suggestions/Extensions exactly fitting our roadmap
Subcontract	<ul style="list-style-type: none">• Small modifications to FAIRDOM Hub• Small extensions
Partnership	<ul style="list-style-type: none">• Continuous development support (as above, but all the time)

Tiers FAIRDOM Hub

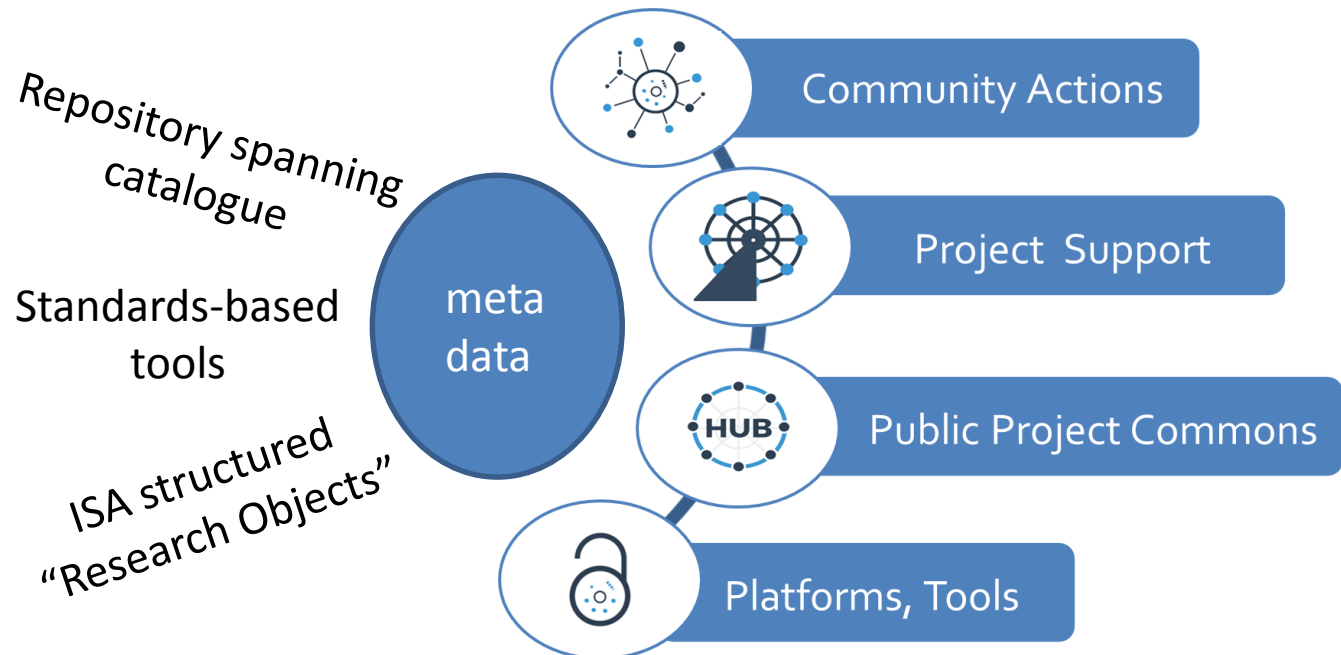
Tier	Proposed
Best effort	<ul style="list-style-type: none">• Use FAIRDOM Hub with small storage requirement• Few support requests (not realistic)
Subcontract	<ul style="list-style-type: none">• Extension for disk space & backup• Support requests beyond „best effort“
Partnership	<ul style="list-style-type: none">• Continuous support

Tiers Community / Service

Tier	Proposed
Best effort	<ul style="list-style-type: none">• Participate in FAIRDOM events on own cost• Proposal of topics for FAIRDOM events• Receiving best effort basis support (limited resources)
Subcontract	<ul style="list-style-type: none">• Pre-call data management webinars• Proposal support• Organise events geared towards ERACoSysMed
Partnership	<ul style="list-style-type: none">• Building PALs program• Collecting requirements• Help in curation• Proposing solutions• Helping with plans• Make plans work• Wider community activities

In summary...Pragmatic FAIR support for projects *people, assets, processes*

- *Multiple, interrelated assets*
- *Multiple, dispersed repositories*
- *Multi-partner, -discipline projects*
- *Multiple community tools*
- *Team science practices*
- *Experiment – Asset lifecycles*
- *Academic innovation drivers*



Developers Foundry Meeting

- **Time:**

December 1st, 10:00

December 2nd, 15:00



- **Location:** **Next to Frankfurt Main Station**

- **Contact:** **wolfgang.mueller@h-its.org**



Working together

Contact mail

- fairdom@fair-dom.org

Web site

- <http://fair-dom.org>

FAIRDOM Hub

- <http://www.fairdomhub.org>



Let's try it - Hands On

