



FAIRDOM for Findable, Accessible, Interoperable, and Reusable Research Data

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CHARME MC meeting & workshop
October 1 -3 2018, Valetta, Malta





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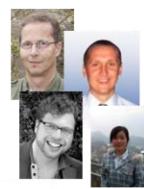
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Standards



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Resources ▾ How To ▾



US National Library of Medicine
National Institutes of Health

PMC



Advanced Journal list

Journal List > PLoS Med > v.2(8); 2005 Aug > PMC1182327



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[PLoS Med.](#) 2005 Aug; 2(8): e124.

Published online 2005 Aug 30. doi: [10.1371/journal.pmed.0020124](https://doi.org/10.1371/journal.pmed.0020124)

PMCID: PMC1182327

PMID: [16060722](https://pubmed.ncbi.nlm.nih.gov/16060722/)

Why Most Published Research Findings Are False

[John P. A. Ioannidis](#)

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SERIES | RESEARCH: INCREASING VALUE, REDUCING WASTE | VOLUME 383, ISSUE 9912, P166-175, JANUARY 11, 2014

Increasing value and reducing waste in research design, conduct, and analysis

Prof John P A Ioannidis, MD • Prof Sander Greenland, DrPH • Prof Mark A Hlatky, MD • Muin J Khoury, MD •

Prof Malcolm R Macleod, PhD • Prof David Moher, PhD • et al. [Show all authors](#)

Published: January 08, 2014 • DOI: [https://doi.org/10.1016/S0140-6736\(13\)62227-8](https://doi.org/10.1016/S0140-6736(13)62227-8) •  [Check for updates](#)



Correctable weaknesses in the design, conduct, and analysis of biomedical and public health research studies can produce misleading results and waste valuable resources. Small effects can be difficult to distinguish from bias introduced by study design and analyses. An absence of detailed written protocols and poor documentation of research is common. Information obtained might not be useful or important, and statistical precision or power is often too low or used in a misleading way. Insufficient consideration might be given to both previous and continuing studies. Arbitrary choice of analyses and an overemphasis on random extremes might affect the reported findings. Several problems relate to the research workforce, including failure to involve experienced statisticians and methodologists, failure to train clinical researchers and laboratory scientists in research methods and design, and the involvement of stakeholders with conflicts of interest. Inadequate emphasis is placed on recording of research decisions and on reproducibility of research. Finally, reward systems incentivise quantity more than quality, and novelty more than reliability. We propose potential solutions for these problems, including improvements in protocols and documentation, consideration of evidence from studies in progress, standardisation of research efforts, optimisation and training of an experienced and non-conflicted scientific workforce, and reconsideration of scientific reward systems.

Box 1. Some Research Practices that May Help Increase the Proportion of True Research Findings

- Large-scale collaborative research
- Adoption of replication culture
- Registration (of studies, protocols, analysis codes, datasets, raw data, and results)
- Sharing (of data, protocols, materials, software, and other tools)
- Reproducibility practices
- Containment of conflicted sponsors and authors
- More appropriate statistical methods
- Standardization of definitions and analyses
- More stringent thresholds for claiming discoveries or “successes”
- Improvement of study design standards
- Improvements in peer review, reporting, and dissemination of research
- Better training of scientific workforce in methods and statistical literacy

www.nature.com/scientificdata

SCIENTIFIC DATA



OPEN

SUBJECT CATEGORIES
» Research data
» Publication characteristics

Comment: The FAIR Guiding Principles for scientific data management and stewardship

Ten Simple Rules for Reproducible Computational Research

Geir Kjetil Sandve^{1,2*}, Anton Nekrutenko³, James Taylor⁴, Eivind Hovig^{1,5,6}

Box 2 | The FAIR Guiding Principles

To be Findable:

- F1. (meta)data are assigned a globally unique and persistent identifier
- F2. data are described with rich metadata (defined by R1 below)
- F3. metadata clearly and explicitly include the identifier of the data it describes
- F4. (meta)data are registered or indexed in a searchable resource

To be Accessible:

- A1. (meta)data are retrievable by their identifier using a standardized communications protocol
- A1.1 the protocol is open, free, and universally implementable
- A1.2 the protocol allows for an authentication and authorization procedure, where necessary
- A2. metadata are accessible, even when the data are no longer available

To be Interoperable:

- I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (meta)data use vocabularies that follow FAIR principles
- I3. (meta)data include qualified references to other (meta)data

To be Reusable:

- R1. meta(data) are richly described with a plurality of accurate and relevant attributes
- R1.1. (meta)data are released with a clear and accessible data usage license
- R1.2. (meta)data are associated with detailed provenance
- R1.3. (meta)data meet domain-relevant community standards

1. For Every Result, Keep Track of How It Was Produced
2. Avoid Manual Data Manipulation Steps
3. Archive the Exact Versions of All External Programs Used
4. Version Control All Custom Scripts
5. Record All Intermediate Results, When Possible in Standardized Formats
6. For Analyses That Include Randomness, Note Underlying Random Seeds
7. Always Store Raw Data behind Plots
8. Generate Hierarchical Analysis Output, Allowing Layers of Increasing Detail to Be Inspected
9. Connect Textual Statements to Underlying Results
10. Provide Public Access to Scripts, Runs, and Results

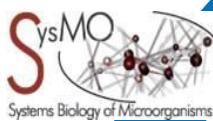
Findable (Citable)
 Accessible (Trackable)
 Interoperable (Intelligible)
 Reusable (Reproducible)



FAIRDOM today



SystemsX.ch
The Swiss Initiative in Systems Biology

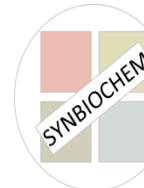


2008



SystemsX.ch
The Swiss Initiative in Systems Biology

RosAge
Reactive oxygen species and
the dynamics of ageing



MANCHESTER
1824
The University of Manchester



Universität
Zürich UZH

ETH Zürich



2010



ISBE

Infrastructure
for Systems Biology
Europe

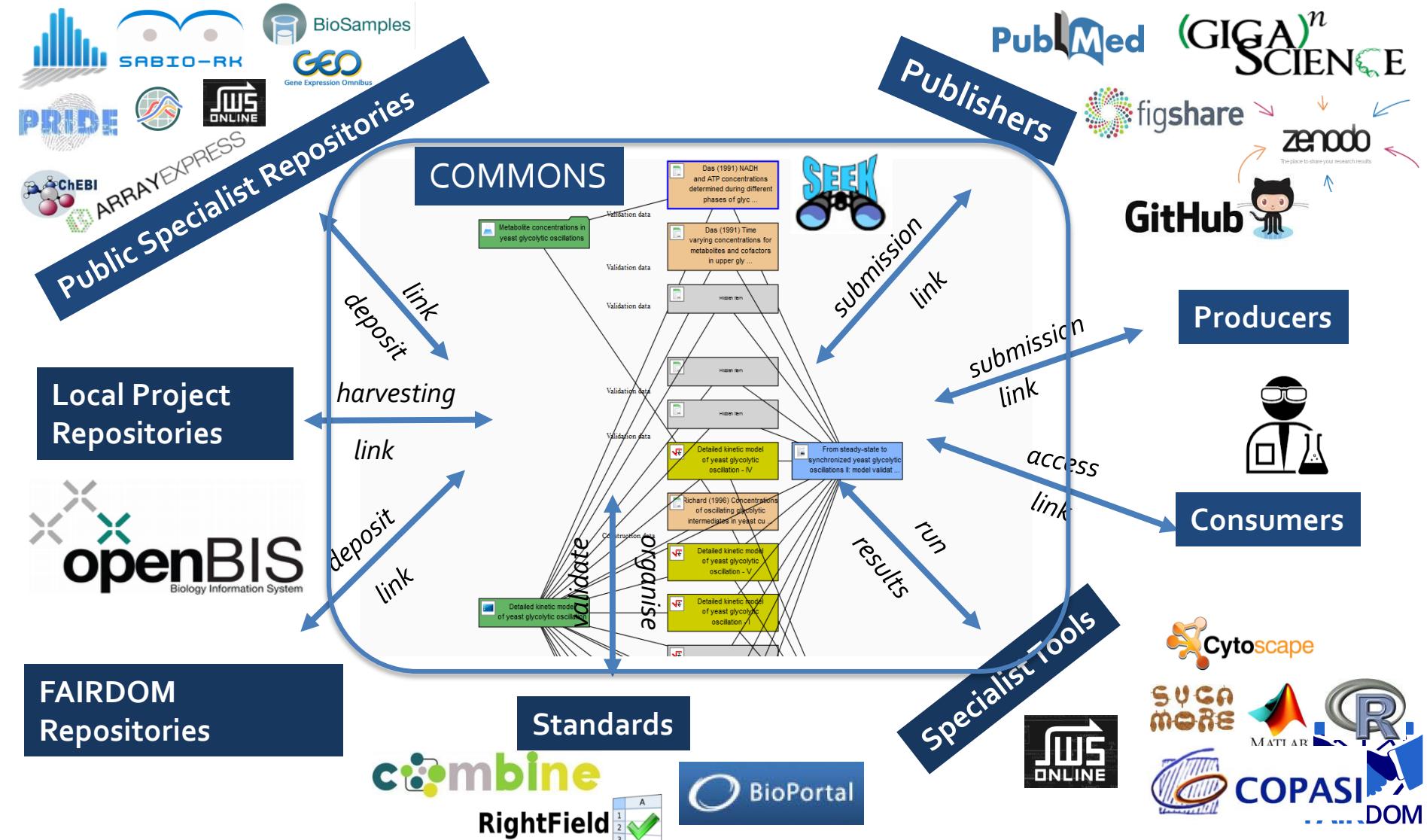
2014



de.NBI
2019



FAIRDOM Platform: Catalogue, Commons, Collections, Project-centric Data Management



FAIRDOMHub

Common Space



Find	– Access – Interoperate – Reuse
Collaborate	– Control – Organise – Retain

- Trusted long-term repository
- Repository space during and after project
- Project controlled spaces
- Working space for projects
- Show space for communicating results
- Collaboration space for partners
- Supp. materials space for publications
- Portal to project on-site repositories
- Portal to modelling tools + public archives
- Shared service



FAIRDOM [Browse](#) [Help](#) Search

Home / Investigations Index / Glucose metabolism in Plasmodium falciparum trophozoites

Glucose metabolism in Plasmodium falciparum trophozoites

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

ID:56

Projects: Whole body modeling of glucose metabolism in malaria patients

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

```

graph TD
    Inv[Investigation: Glucose metabolism in Plasmodium falciparum trophozoites] --> S1[Study: Model construction]
    Inv --> S2[Study: Model validation]
    Inv --> S3[Study: Model analysis]
    Inv --> P[Publication: Construction and validation of a detailed kinetic model of glycolysis in Plasmodium]
    
    S1 --> A[Analysis: Modelling Analysis: PFK]
    S2 --> A
    S3 --> A
    
    A --> M[Model: PFK Kinetic model]
    A --> SOP[SOP: PFK Kinetic characterisation]
  
```

Study

- Study: Model construction
- Study: Model validation
- Study: Model analysis

Investigation

Investigation: Glucose metabolism in Plasmodium falciparum trophozoites

Publication: Construction and validation of a detailed kinetic model of glycolysis in Plasmodium

Related Items

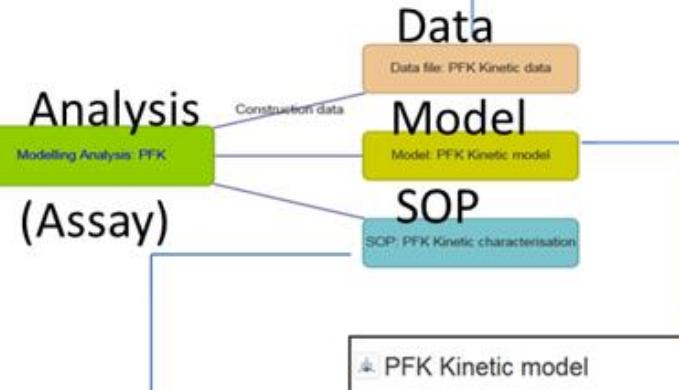
- People (1)
- Projects (1)
- Studies (3)
- Assays (24)
- Data files (16)
- Models (13)
- SOPs (13)
- Publications (1)

David Van Niekerk

Projects: SystemCDB, Whole body modeling of glucose metabolism in malaria patients
Institutions: University of Thessaloniki

Disciplines: Modeler
Roles: Not specified
Expertise: Not specified
Tools: Not specified

Variables		Values (measured)				
Assay ID	PFK-Kinetic Data					
Category	None					
Category SEED ID						
Project						
Sample ID						
Assay Type	PFK					
Assay Date						
Assay Time						
Assay Location						
Description	kinetics measurement					
Experimental						
Experiments						
Performance (approx.)						
Experimental_conditions						
Condition	Incubation	pH	Biotin	Biotin	Biotin	Biotin
Compound (concentration)		7.4	0.001	0.001	0.001	0.001
Conc			0.001	0.001	0.001	0.001
Conc_label (approx.)						
End_Conc (approx.)						
Enzyme						
Enzyme_group	Biotin					
INCUBATION CONDITIONS						
Incubation	Incubation	ATP	ATP	ATP	ATP	ATP
Conc	0.001	ATP	ATP	ATP	ATP	ATP
Conc_label (approx.)						
Incubation_time (approx.)	4.5 (44.5)	0	0	0	0	0
Incubation_time_label (approx.)						
PFK (approx.)	10	0	0	0	0	0



PFK Kinetic model

Mathematica notebook for the parameterisation of the PFK rate equation based on SEED data.

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

- PFK-SEED.RD (Mathematica notebook - 302 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)

$$\frac{V_{PFK} \cdot \frac{s_{IP}}{K_{ATP}} \cdot \frac{s_{BP}}{K_{PFK}}}{(1 + \frac{s_{IP}}{K_{ATP}}) \cdot (1 + \frac{s_{BP}}{K_{PFK}} + \frac{s_{BP}}{K_{PFKE}}) \cdot (1 + \frac{s_{IP}}{K_{ATP}} + \frac{s_{IP}}{K_{ATPE}})}$$

Selected item: Model: PFK Kinetic model

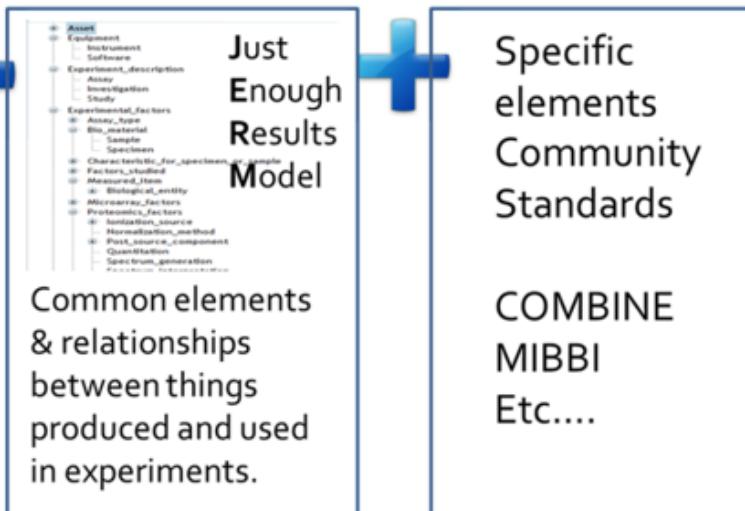
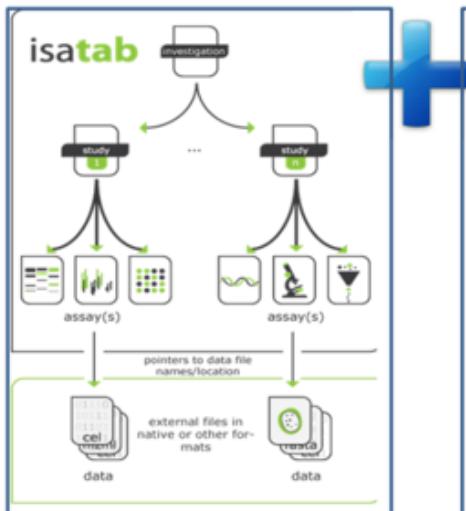
PFK Kinetic model

Specific activity of the glycosome enzyme were measured in microtiter plate assays that were adapted from a previously published protocol (13). The reaction mixture contained 20 mM Tris-HCl, 1 mM EGTA, 1 mM DTT, 1 mM Biotin, 1 mM Pyruvate kinase, 1 mM ADP, 1 mM Phosphoenolpyruvate (PEP), 1 mM NADH and 10 mM NaF. The reaction mixture (100 μl) was incubated at 37°C for 30 min. The production of ATP by the oxidation of NADH (0.8 mM) via LDH, PK in the presence of biotin and PEP was measured at 340 nm. The specific activity rates could not be measured to maximal specific activity at saturating substrate concentrations. A control rate was determined at 1.25 mM ADP and 1 mM PEP.

[1] Neuraut R, Pessaggi L, Reijnen C, Engelsma E, van der Weijden C, et al. (2006) Can yeast glycolysis be understood in terms of its cellular context? Biochem J 399:511-520.

[2] Wijnrich S, Sanchez C, Gode H, Grossz-Wittmann L, Werner J, et al. (2006) Differential stimulation of the Na⁺/H⁺ exchange determines ion homeostasis in Plasmodium falciparum. J Cell Sci 119:325-335.

Aggregation and scientific context. The Investigation, Studies, Assays (**ISA**) framework is used to allow research assets and experimental background to be aggregated and interlinked; providing descriptions, scientific context, relationships between assets, and includes clear credit to the scientists and projects involved.



Specific
elements
Community
Standards

COMBINE
MIBBI
Etc....

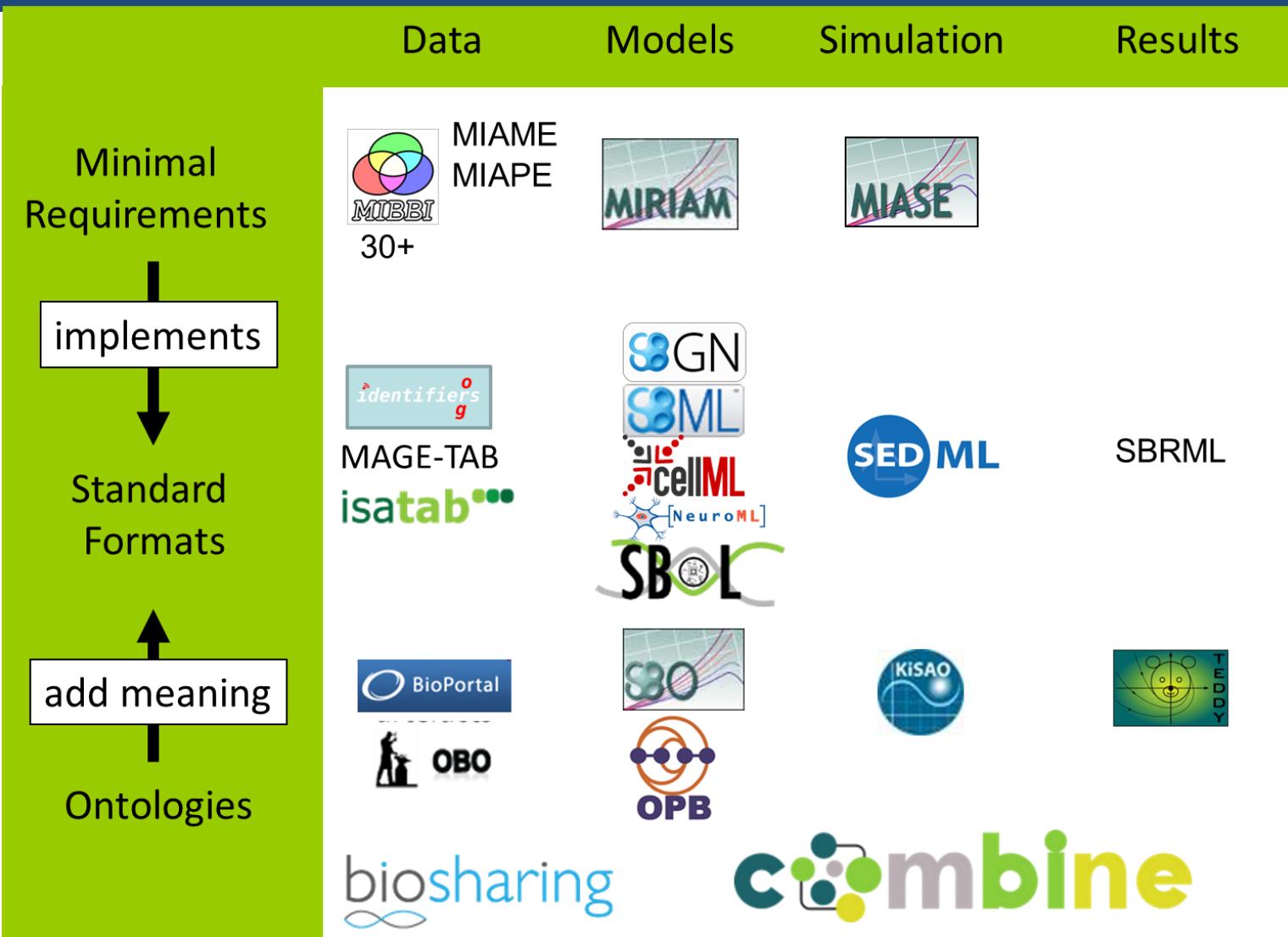


Spreadsheet tooling for metadata
templates and metadata harvesting

RightField, for embedding ontology term selection into spreadsheets, enabling JERM compliant annotation of data.

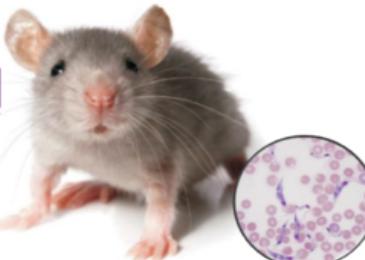
<http://www.rightfield.org.uk>

Standards



Biosamples in SEEK

miniMECH-Trypo

	A	C	D	E	F	G	H	I	J
1	Add a New Paper	Save Paper Review	Score Paper Review	Show All PaperReview	17066074	Load			
2									
3					Paper #	Paper #	Paper #	Paper #	
4					84%	84%	58%	92%	
5					93%	93%	100%	93%	
6					100%	100%	100%	100%	
7					92%	92%	87%	95%	
8									
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Process = $\frac{\text{Interest}}{\text{Friction}} \times \text{Number people reach}$

The Neylon Equation

Information about the host	18	Is the age of the animal described? (e.g. 6-8 weeks old)	21	Protocol Parameters
	19	Is the gender of the animal described? (e.g. Female)	22	SDRF File
Animal	20.1	Is the housing conditions -light/dark cycle- described? (e.g. 12 hours light/12 dark)	23	data file
	20.2	Is the housing conditions -temperature- described? (e.g. 25 °C)	24	ADF file
	20.3	Is the housing conditions -humidity- described? (e.g. 40-45 %)	25	Term Source Name
	20.4	Is the housing conditions -food/water access- described? (e.g. limited)	26	Term Source File
	20.5	Is the housing conditions -animals per cage- described? (e.g. 3 mice)	27	Term Source Version
	20.6	Is the housing conditions -sex cage- described? (e.g. same-sex cage)	28	software_manufacturer
	21	Is the method of sacrifice described? (e.g. Cervical dislocation)	29	submitter
	22	Is the cell type identified? (e.g. HEK 293)	30	files/MGEC
	23	In primary culture, is the organ/tissue from which cells come identified?	31	date
	24	In primary culture, is the method of purification of the cells described?	32	integer
			33	text
			34	text
			35	text
			36	text
			37	text
			38	text
			39	text
			40	text
			41	text
			42	text
			43	text
			44	text
			45	text

RightField

A
1
2
3

IDFExcelExample | SampleData | values | +



Clinical Data → Many Centers, Many Formats

Clinical Data Homburg (Lammert)

Code	DoB	Sex	Ethnicity	Inclusion date	Age	Any NOD2-mutation	p.R702W	p.G908R	c.3020 insC	K	MELD	Child-Pugh	Cirrhosis	Etiology cirrhosis	Compensated/decompensated	Date Decompensation (most actual)	Time decompensation to Inclusion (days)	HE actual/prior	Date last HE	Time decompen	Varices	Variceal bleeding actual/prior	Date variceal
							3 WT 2 HET 3 HOM	1 WT 2 HET 3 HOM	1 WT 2 HET 3 HOM	Diabetes mellitus													

Clinical Data Charité Berlin (Hudert)

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W
1	Patient data	Study ID	Gender	Age	Height	Weight	BMI	BMI-SDS	Waist	Hip	Histology	(Grading and Staging according to NASH CRN System)	Chemistry									
2			1=male, 2=female	years	cm	kg	kg/m ²		cm	cm	Staging	Grading	ALT U/l	AST U/l	GGT U/l	PCHE kU/l	GLDH U/l	Bile Acids umol/l				
3											Fibrosis	NAS	portal	lobular	Inflammation	Inflammation	Ballooning					
4											Steatosis											

Clinical Data Dresden (Hampe)

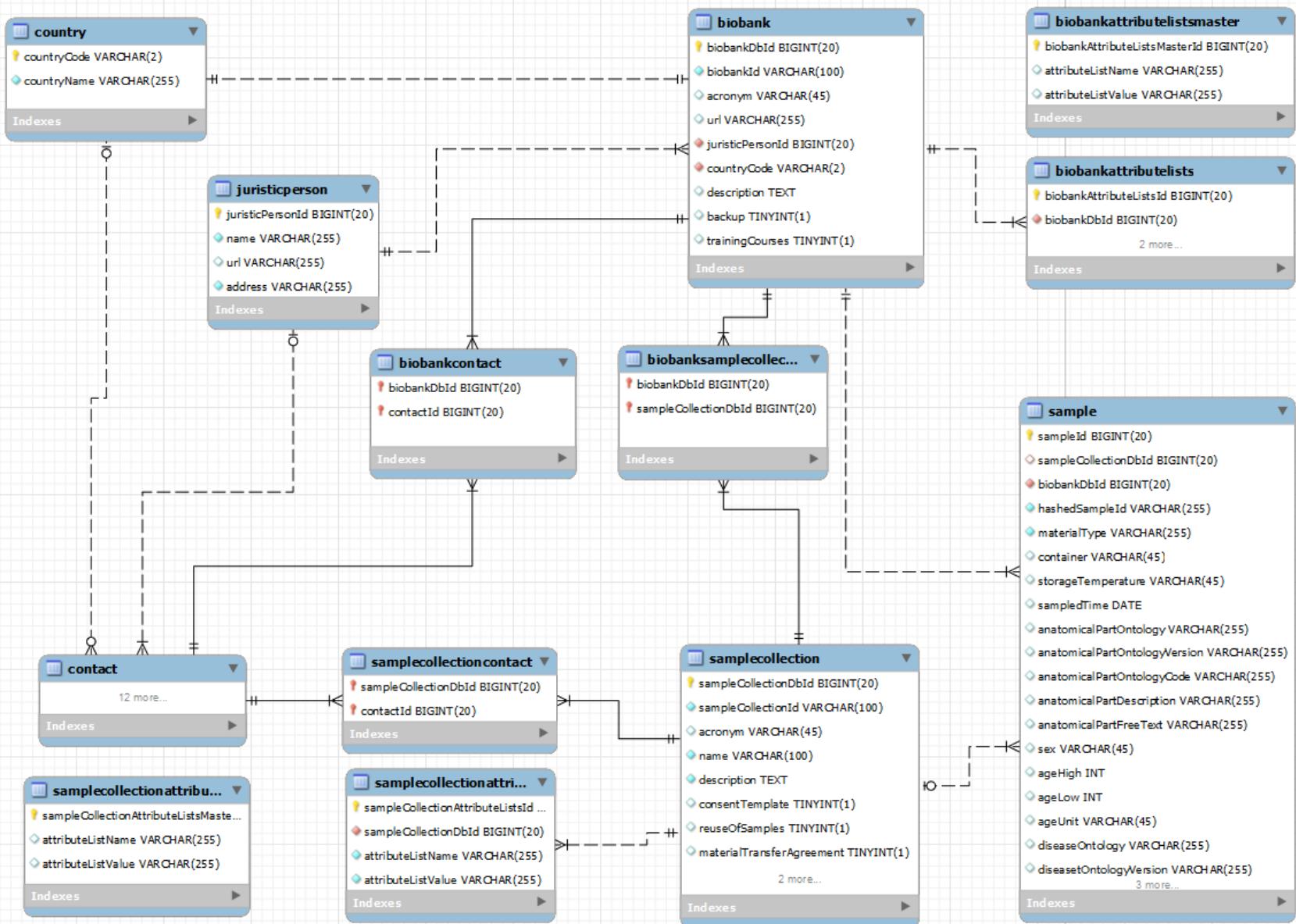
A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W
1	PAT.ID	PROCESS	GRUPPE	BARI	SEX	NAS	NAS.FAT	NAS.BALLOONING	NAS.ENTZ	Verfettung	Entzündung	Fibrose	AGE	Gewicht	BMI	Diabetes	OP.TYP	gGT (U/l)	AP (U/l)	Ges. Bilirubin (mg/dl)	ALT (U/l)	
2	6503	BIL_2		3	1	2	1	1	0	0	25	1	0	41	198	54,3	1	1	21	84	0,36	
3	6503			3	1	2	1	1	0	0	25	1	0	41	198	54,3	1	1	21	84	0,36	
4	6610	BIL_2		3	1	1	3	2	1	0	50	1	0	41	185	59,7	2	2	81	90	0,43	

Mapping the different data formats to create one consolidated spreadsheet template of description data (describing donor attributes) for human clinical samples in LiSyM



Standardized Sample Description: MIABIS

Minimum Information About Blobank Data Sharing



Standard Operating Procedures

Quality Control

[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

[Download SOP](#)[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

None

Filename: Lentiviral production and infection_SOP_04042011.pdf

Format: PDF document

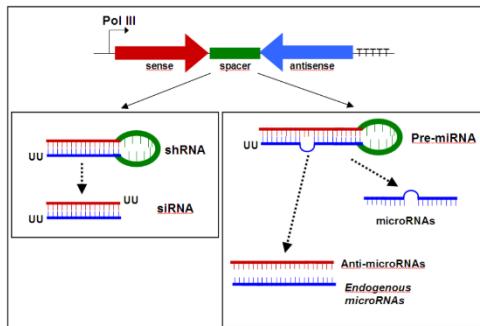


Fig.1: Schematic presentation of designed template sequences which are processed intracellularly into short hairpin RNAs, microRNAs or anti-microRNAs. The stem-loop structures consisting of both the sense and anti-sense strands of the targeted sequence are separated by a loop sequence.

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)

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 $3,5 \times 10^5$ cells per 1 T175 flask in 30 ml of medium with components and G148 to achieve optimal phase of cellular growth.



Reproducible models in FAIRDOM

metadata annotation against standards
validation, comparison and simulation

JWS Online

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

Schema Time evolution Steady-state Parameters

Reactions Parameters Fixed species Initial values Functions and Rules Events Constraints

Simulate Steady State Analysis? (Simulate)

Save as new version Model format: SBML Save

Validate Check

Annotator Annotate

BiVes

Download schema

SBML Model simulation

The screenshot shows a complex reaction network diagram with various species and reactions. A central feature is a large green circle labeled 'vPFvGLYfr'. Other nodes include 'iEX', 'vPFvGLOfr', 'vPFvHK', 'vPFvPPK', 'vPFvVALD', 'vPFvGAPDH', 'vPFvPDK', 'vPFvPGM', 'vPFvLDH', 'vPFvATPase', 'vPFvPK', 'vPFvENO', and 'C00092'. A legend on the right indicates that deletions are red and insertions are blue. Simulation parameters include 'Gravity' (checkbox), 'Repulsion' (checkbox), 'Pool threshold' (set to 4), and 'Species' and 'Reactions' pinned/unpinned buttons. A large 'JWS ONLINE' logo is prominently displayed in the center.

Model comparison

The screenshot shows a reaction network diagram with nodes 'vv2', 'vv3', and 'p'. Below the diagram are validation tools: 'Check' (checkbox), 'Create derivative' (button), and 'Download' (button). A 'Figure A1 pJAK2' plot is shown to the right, comparing experimental data (red dots) with a simulation (blue line).

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

Deletions are coloured in red and insertions are coloured in blue

SBML Differences

Both documents have same Level/Version: L3V1

Parameters

VappSPSSP 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

Model versioning

Reproducing simulations

JWS Online Model Database Simulate

SED-ML Simulation Result: bachmann2011

Details Download Create derivative

Figure A1.pJAK2

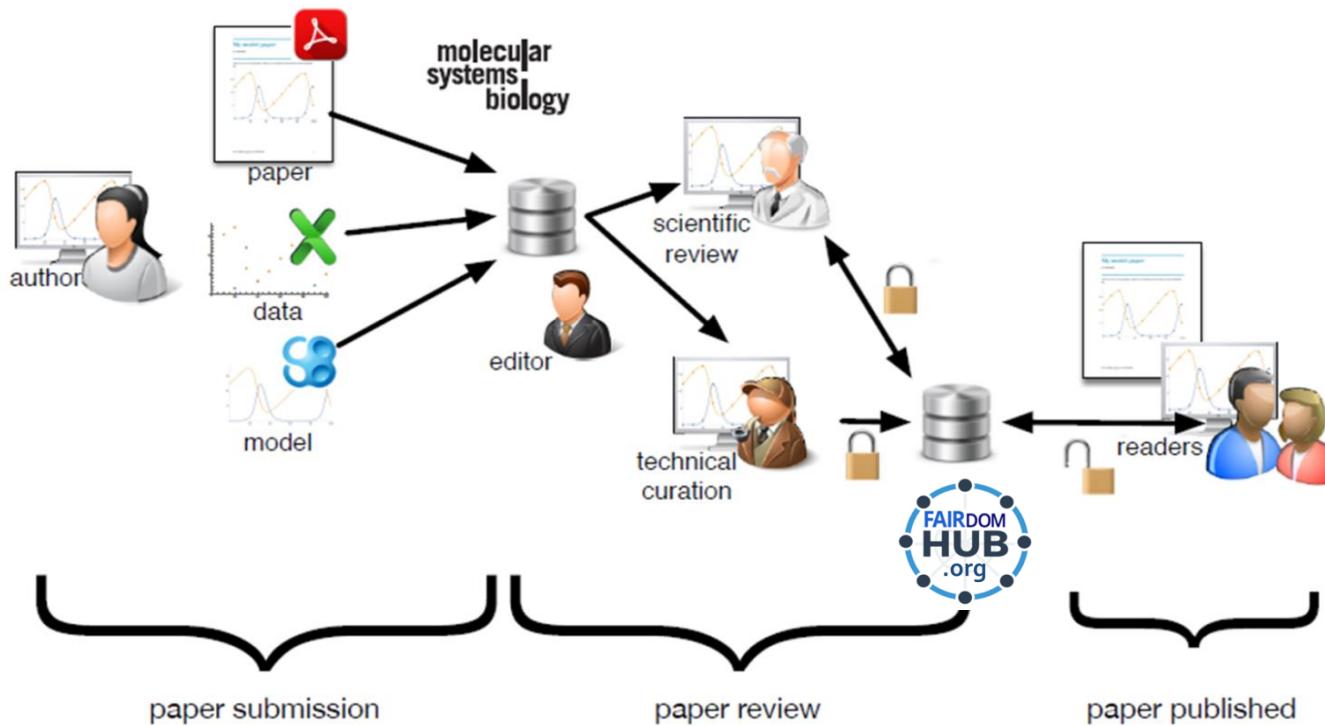
Figure A1 pJAK2

The screenshot shows a line graph titled 'Figure A1 pJAK2'. The x-axis is 'time' (0 to 250) and the y-axis is concentration (0.0 to 1.0). Experimental data points are shown as red dots, and a simulation is shown as a blue line. The plot is titled 'Figure A1 pJAK2'.

SED ML

FAIRDOM service : model curation

- * store DOI citable supplementary files on FAIRDOMHub
- ** model and data curation
- *** reproducible clickable figures in papers using SED-ML



Credit and Attribution

Citing FAIRDOM Entries, living and snapshot entries, contributors



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

Keywords

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

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

doi:10.1111/febs.13237

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, 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, glyceral; HK, hexokinase; LAC, lactate; LDH, lactate dehydrogenase; MCT, monocarboxylate transporter; ODE, ordinary differential equation; PEP, phosphoenolpyruvate; PK, 6-phosphofructokinase; PGK, 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.

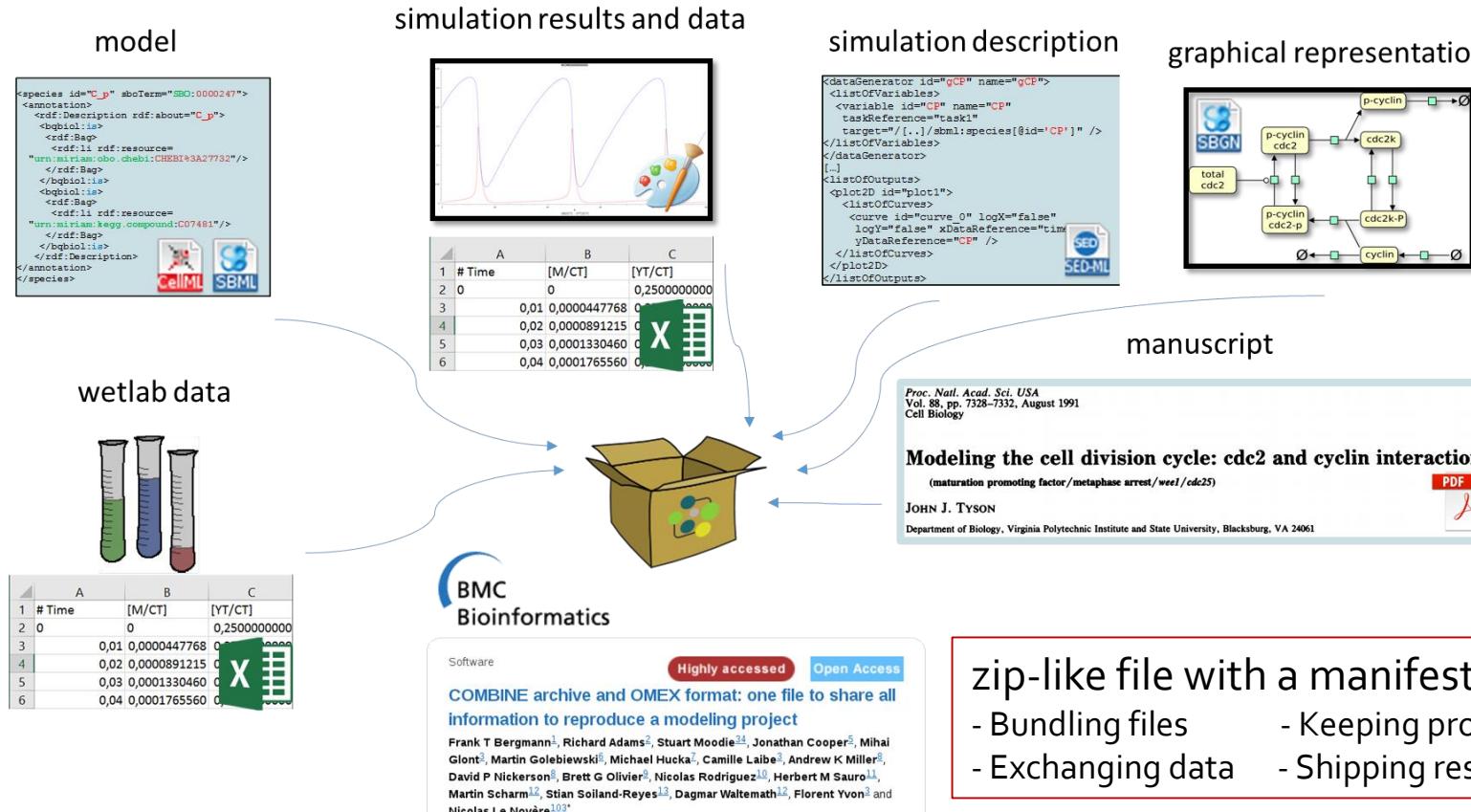
Penkler et al (2015) FEBSJ 282:1481–1511
<https://dx.doi.org/10.1111/febs.13237>

The screenshot shows the FAIRDOM platform interface. At the top, there is a search bar and navigation links for 'Browse', 'Documentation', 'Search here...', 'Search', and 'Contributors'. Below the header, a breadcrumb trail indicates the current page: 'Home / Investigations Index / Glucose metabolism in *Plasmodium falciparum* trophozoites'. The main title is 'Glucose metabolism in *Plasmodium falciparum* trophozoites'. A brief description states: '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.' Below this, a graph diagram shows the relationship between 'Glucose metabolism in Plasm...' (highlighted in yellow), 'Model validation' (green box), and 'Model construction' (green box). On the right side, there are sections for 'Contributors' (with a photo of a person), 'Activity' (Views: 326, Created: 8th Aug 2014 at 15:16, Last updated: 11th Dec 2014 at 09:55), and a large 'doi' logo. At the bottom, a URL is provided: <https://doi.org/10.15490/seek.1.investigation.56>.



Packaging: CombineArchive

<https://sems.uni-rostock.de/projects/combinearchive/>



zip-like file with a manifest & metadata

- Bundling files
- Keeping provenance
- Exchanging data
- Shipping results

Scharn M, Wendland F, Peters M, Wolfien M, Theile T, Waltemath D
SEMS, University of Rostock

Bergmann, F. T., Adams, R., Moodie, S., Cooper, J., Glont, M., Golebiewski, M., ... & Olivier, B. G. (2014). COMBINE archive and OMEX format: one file to share all information to reproduce a modeling project. *BMC bioinformatics*, 15(1), 1.



More than 200 curated SED-ML simulations, each reproducing a publication figure

The screenshot shows a web browser window for the JWS Online platform. The URL in the address bar is `jjj.bio.vu.nl`. The page title is "SED-ML Simulation database". On the left, there are two tabs: "Curated Simulations" (selected) and "Session Simulations". Below these tabs is a section titled "Simulation" containing a list of simulation names. Each name is followed by a "Download" button with a green play icon. On the right side of the page is a "Filters" sidebar with fields for "Name" and "Model Name", and buttons for "Filter" and "Clear". At the bottom of the main content area is a navigation bar with page numbers from 1 to 8, where 8 is highlighted in blue.

Simulation	Action
tripathi2007_Fig7_8to7_9	Download
valero2006_Fig1AandB	Download
vanHeerden2014_Fig1B	Download
vanHeerden2014_Fig4	Download
wahl2000_Fig6	Download
wang2012_Fig1and2	Download
wang2015_Fig9	Download
wodarz2000_Fig2	Download
wodarz2007_Fig1	Download
zhao2013_Fig3A	Download



Direct simulation of SED-ML files in SEEK, links model (e.g. JWS) and experimental data files (e.g. SEEK) to reproduce manuscript figures

The screenshot shows a web browser window with the following details:

- Header:** Safari, File, Edit, View, History, Bookmarks, Window, Help.
- Address Bar:** fairdomhub.org
- FAIRDOM HUB Navigation:** Home, Browse, Help, Search, Register, Log in.
- Breadcrumbs:** Home / Studies Index / Figure 1C: Biphasic control can resist mutant invasion of feedback circuits.
- Title:** **Figure 1C: Biphasic control can resist mutant invasion of feedback circuits.**
- Description:** C Trajectories of Z from different initial concentrations of cells (Z) (i) or y (ii) for the circuit of (B). The healthy concentration $Z = ZST$ is reached regardless of initial concentration of Z, as long as it is nonzero, and regardless of the initial concentration of y.
- SED-ML simulation:** https://ijj.bio.vu.nl/models/experiments/karin2017_fig1c/simulate
- SEEK ID:** <https://fairdomhub.org/studies/383>
- Investigation:** Karin et al (2017) Molecular Systems Biology
- Projects:** Molecular Systems Biology
- Person responsible:** Jacky Snoep
- Experimentalists:** Not specified
- Contributor and Creators:** (Profile picture)
- Activity:**
 - Views: 154
 - Created: 31st Jul 2018 at 11:51
 - Last updated: 31st Jul 2018 at 12:05
- Graph View:** A network diagram showing nodes and connections. Nodes include "Figure 1C Biphasic control can resist mutant invasion of feedback circuits.", "Biphasic control can resist mutant invasion of feedback circuits.", "Karin et al (2017) Molecular Systems Biology", and several gray square nodes. A legend on the left shows icons for zoom, rotate, and selection.

API search example in Mathematica

Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help

Untitled-1

```
(*a search example, including the search_type category*)
query = "Snoep";
url = "https://fairdomhub.org/";
Dataset[URLExecute[url <> "search", {"q" \[Rule] query, "search_type" \[Rule] "publications", "format" \[Rule] "json"}, {"RawJSON"}]][[1]]
```

Out[=]

id	type	attributes	links
		title	self
196	publications	Reproducible computational biology experiments with SED-ML--the Simulation Exper`.	/publications/196
250	publications	Design principles of nuclear receptor signaling: how complex networking improves `.	/publications/250
195	publications	Emergence of the silicon human and network targeting drugs	/publications/195
176	publications	From steady-state to synchronized yeast glycolytic oscillations I: model construction	/publications/176
175	publications	From steady-state to synchronized yeast glycolytic oscillations II: model validation	/publications/175
174	publications	Sustained glycolytic oscillations in individual isolated yeast cells	/publications/174
240	publications	Construction and validation of a detailed kinetic model of glycolysis in `.	/publications/240
268	publications	Targeting glycolysis in the malaria parasite Plasmodium falciparum	/publications/268
381	publications	From steady-state to synchronized yeast glycolytic oscillations II: model validation.	/publications/381
382	publications	From steady-state to synchronized yeast glycolytic oscillations I: model construction.	/publications/382
375	publications	Allosteric regulation of phosphofructokinase controls the emergence of glycolyt`.	/publications/375
379	publications	Sustained glycolytic oscillations in individual isolated yeast cells	/publications/379
378	publications	Heterogeneity of glycolytic oscillatory behaviour in individual yeast cells	/publications/378
213	publications	Intermediate instability at high temperature leads to low pathway efficiency for `.	/publications/213
384	publications	Biphasic response as a mechanism against mutant takeover in tissue homeostasis circuits	/publications/384
383	publications	Frequency doubling in the cyanobacterial circadian clock	/publications/383
194	publications	A mathematical modelling approach to assessing the reliability of biomarkers of `.	/publications/194
269	publications	Quantitative analysis of drug effects at the whole-body level: a case study for `.	/publications/269
139	publications	RightField: embedding ontology annotation in spreadsheets	/publications/139
180	publications	Stealthy annotation of experimental biology by spreadsheets	/publications/180

K < showing 1–20 of 24 > K

Packaging: Research Objects



Enabling **reproducible**, transparent research.



Standards-based metadata framework for
bundling (scattered) resources with context and citation



Use a workflow – the vision!

preferably a workflow management system

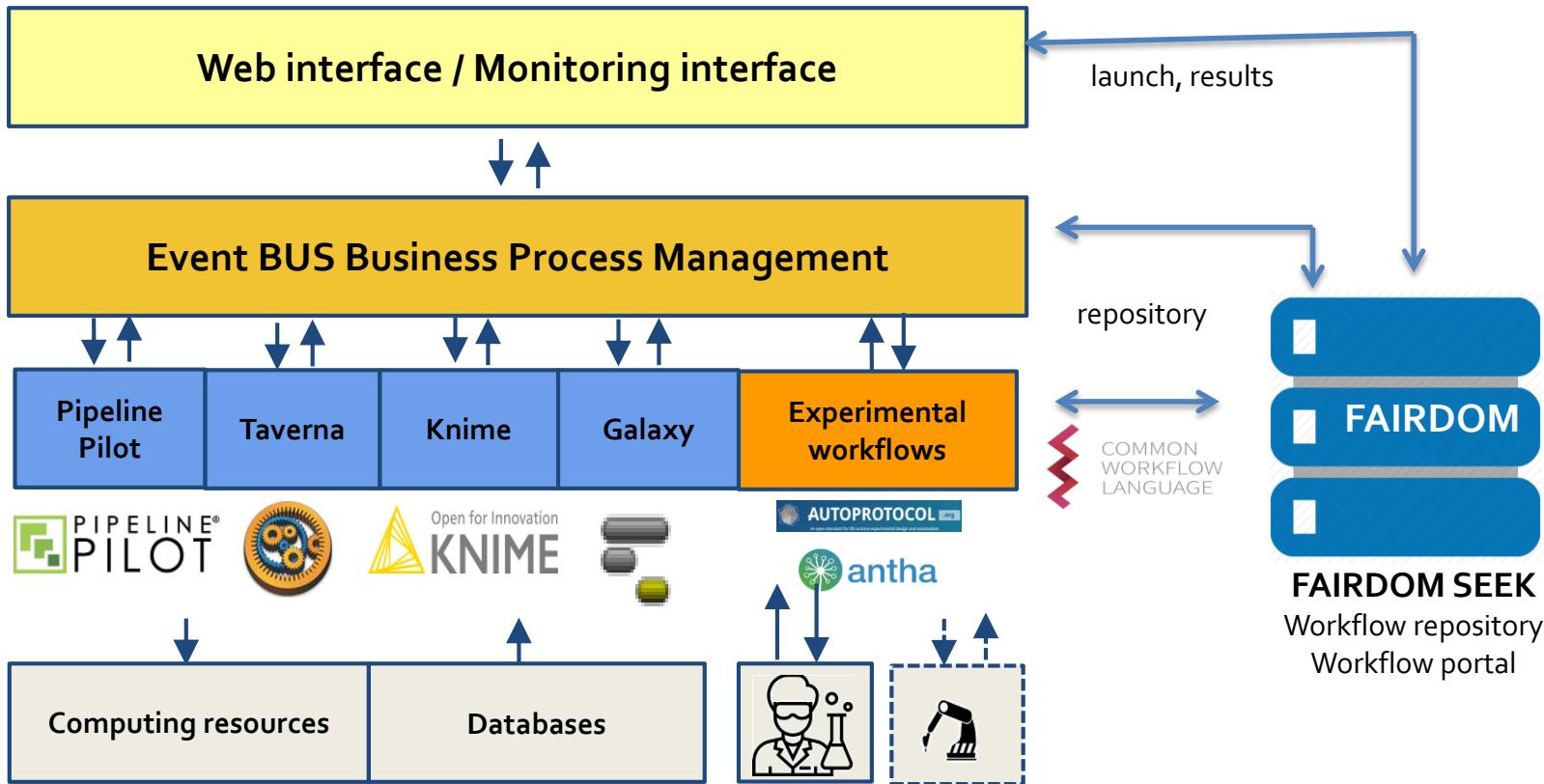
preferably described using Common Workflow Language

Front-end

Workflow
BPM layer

Workflow
Computation
Application
layer

Effector
layer



FAIRDOM support

Understanding the project, its collaborations, its assets, and its workflows

Helping projects promote their project, skills and results



Maintaining, archiving and securing access to FAIRDOMHub



Customising on-site project installations



Managing, developing and updating the platforms and tools



Designing and deploying the technical platforms and the right tools



Working with researchers and technicians to design and adopt practices and procedures and curate models and data.



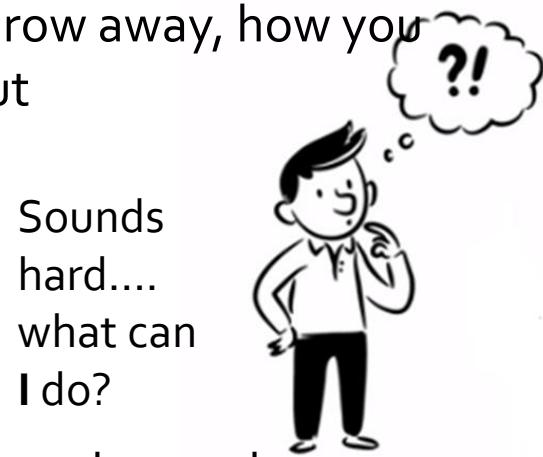
Training researchers and students



12 steps to being FAIR

plan to be born FAIR

1. plan data management lifecycle: plan, cost and implement pathways and storage including what you will archive, what you will throw away, how you will collect metadata and how you will curate throughout
2. use standard identifiers and identifier standards
3. use metadata standards with data provenance
4. catalogue / register data with metadata
5. have access and sharing policies with licenses
6. use data (assets) management platforms and tools that work together
7. deposit into public archives
8. have a sustainability / end project plan
9. resource and support, and that also means people too
10. embed data management into work practices and do some training
11. give credit
12. check if you have sensitive data issues



Sounds
hard....
what can
I do?

We are part of/liaising with numerous initiatives



Coordinating Action Systems Medicine
Implementation of Systems Medicine across Europe

