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HITS

How to Share FAIR – The FAIRDOM Data and Model Management Practice

Martin Golebiewski, Maja Rey, Wolfgang Müller
HITS gGmbH (Heidelberg, Germany)

7th Conference on Systems Biology of Mammalian Cells (SBMC 2018), Bremen July 4th, 2018

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GERMAN NETWORK FOR BIOINFORMATICS INFRASTRUCTURE
ERASysAPP
ERA-Net for Applied Systems Biology
LiSyM
Liver Systems Medicine
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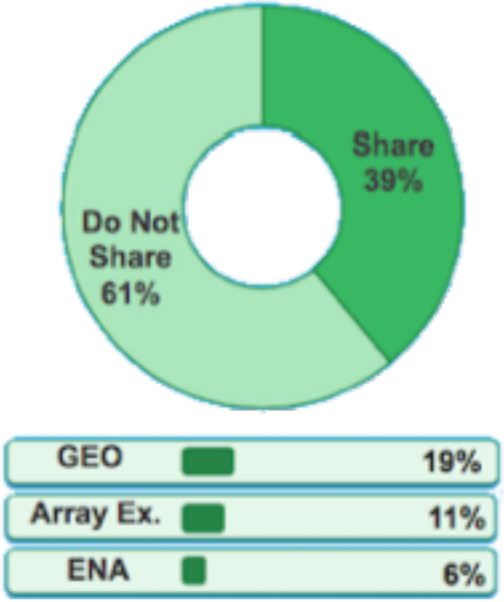
Tutorial Agenda July 4th 2018

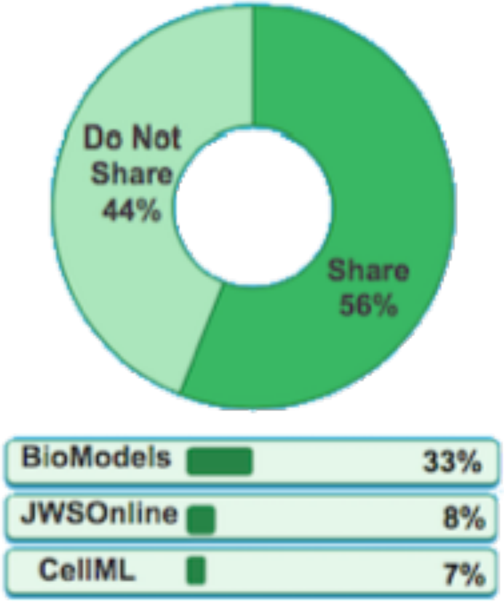
9:00 – 9:10	Welcome and tour de table
9:10 – 9:30	FAIRDOM introduction
9:30 – 9:45	Introduction into SABIO-RK
9:45 – 10:10	SEEK hands on
10:10 – 10:30	Coffee break
10:30 – 11:15	Modelling SEEK hands on
11:15 – 11:45	Programmatic access to SEEK
11:45 – 12:00	Wrap up

Many researchers do not share their data or models in open repositories

Data



Models



*top three most popular

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

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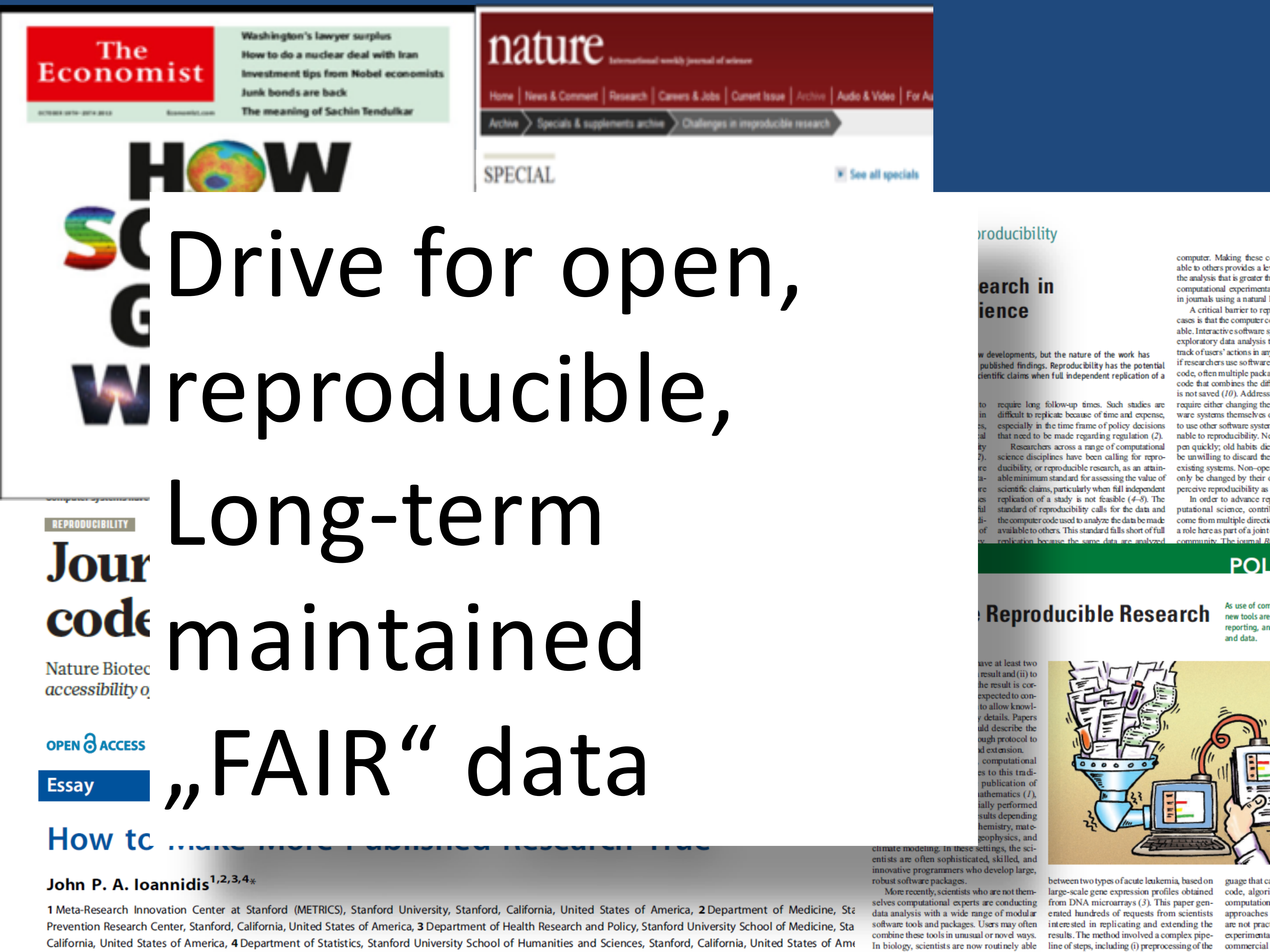

Drive for open, reproducible, Long-term maintained „FAIR“ data

The Economist

Washington's lawyer surplus

How to do a nuclear deal with Iran

Investment tips from Nobel economists

Junk bonds are back

The meaning of Sachin Tendulkar

nature International weekly journal of science

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Archive > Specials & supplements archive > Challenges in irreproducible research

SPECIAL

See all specials

REPRODUCIBILITY

Nature Biotec

OPEN ACCESS

Essay

How to Make More Published Research True

John P. A. Ioannidis[1,2,3,4]*

1 Meta-Research Innovation Center at Stanford (METRICS), Stanford University, Stanford, California, United States of America, 2 Department of Medicine, Sta Prevention Research Center, Stanford, California, United States of America, 3 Department of Health Research and Policy, Stanford University School of Medicine, Sta California, United States of America, 4 Department of Statistics, Stanford University School of Humanities and Sciences, Stanford, California, United States of Ame

require long follow-up times. Such studies are difficult to replicate because of time and expense, especially in the time frame of policy decisions that need to be made regarding regulation (2).

Researchers across a range of computational science disciplines have been calling for reproducibility, or reproducible research, as an attainable minimum standard for assessing the value of scientific claims, particularly when full independent replication of a study is not feasible (4–8). The standard of reproducibility calls for the data and the computer code used to analyze the data be made available to others. This standard falls short of full replication because the same data are analyzed

Reproducible Research

climate modeling. In these settings, the scientists are often sophisticated, skilled, and innovative programmers who develop large, robust software packages.

More recently, scientists who are not themselves computational experts are conducting data analysis with a wide range of modular software tools and packages. Users may often combine these tools in unusual or novel ways. In biology, scientists are now routinely able

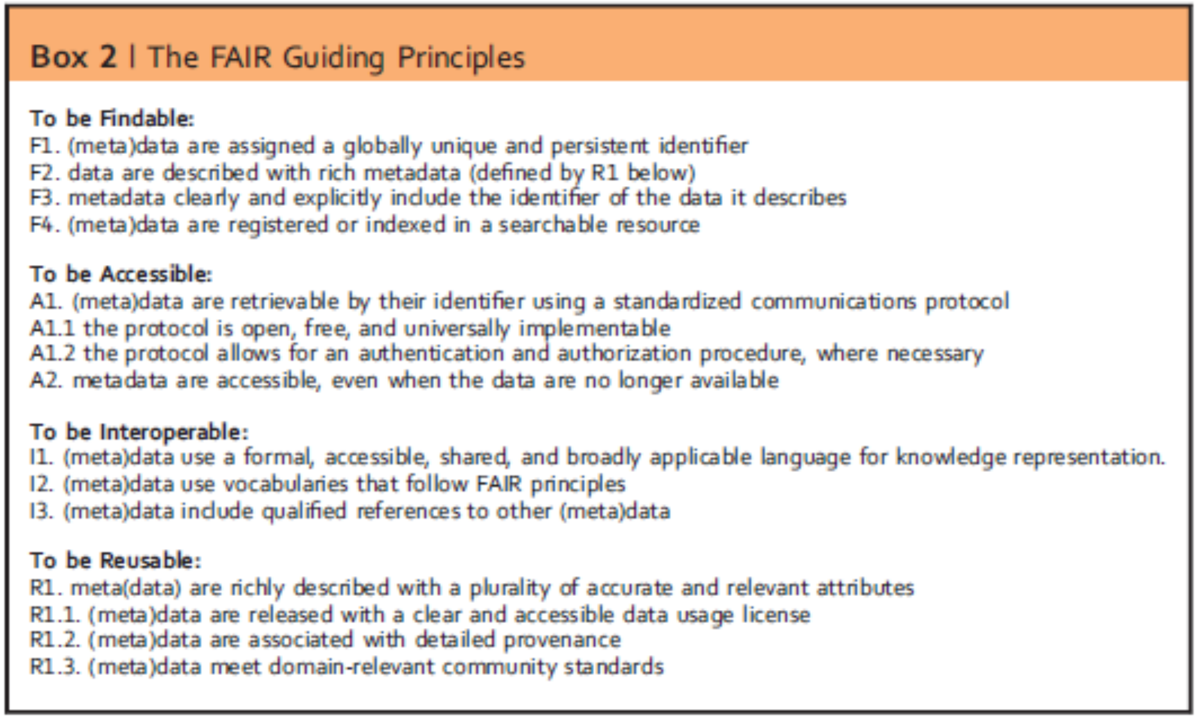
between two types of acute leukemia, based on large-scale gene expression profiles obtained from DNA microarrays (3). This paper generated hundreds of requests from scientists interested in replicating and extending the results. The method involved a complex pipeline of steps, including (i) preprocessing of the

How to Share Data FAIR ?


SCIENTIFIC DATA

OPEN

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


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

SCIENTIFIC DATA (2016), 3: 160018

https://www.force11.org/group/fairgroup/fairprinciples

Findable

Accessible

Interoperable

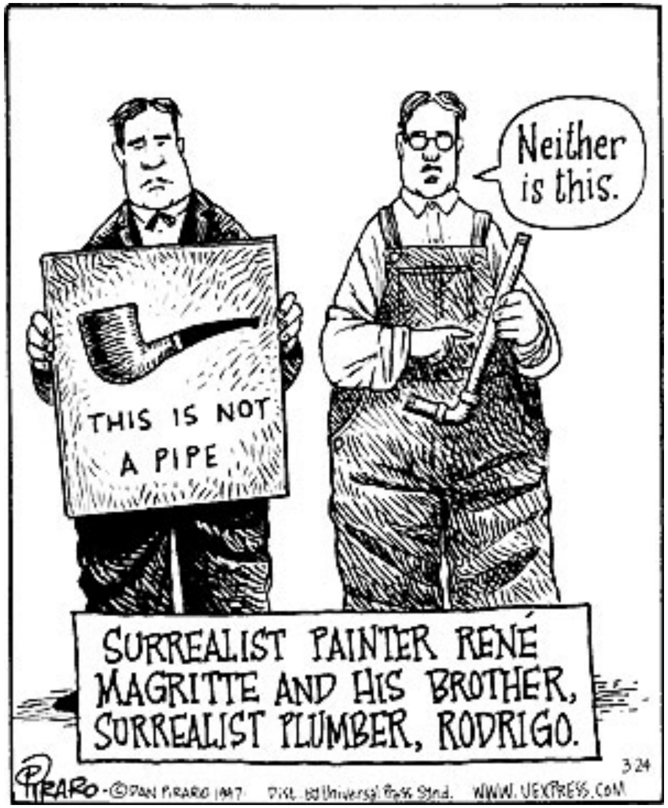
Reusable

Data

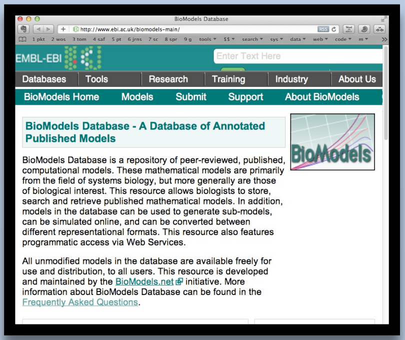
Operations

Models

Data representation needs standardized formatting and description



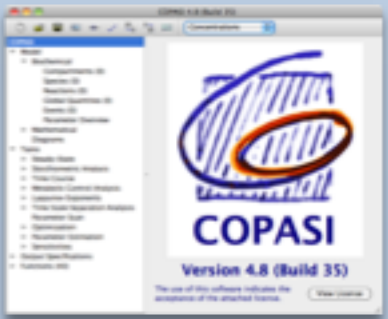
Modelers often use several software tools

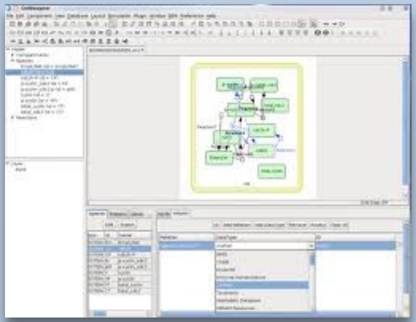


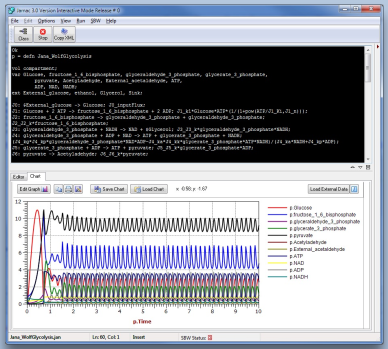
BioModels Database - A Database of Annotated Published Models

BioModels Database is a repository of peer-reviewed, published, computational models. These mathematical models are primarily from the field of systems biology, but more generally are those of biological interest. This resource allows biologists to store, search and retrieve published mathematical models. In addition, models in the database can be used to generate sub-models, can be simulated online, and can be converted between different representational formats. This resource also features programmatic access via Web Services.

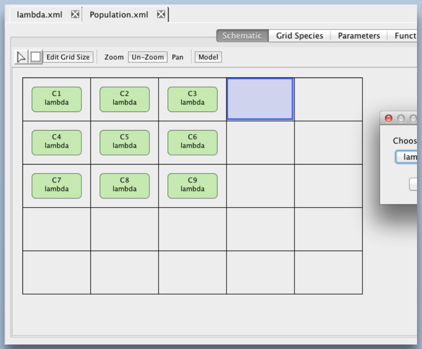
All unmodified models in the database are available freely for use and distribution, to all users. This resource is developed and maintained by the BioModels.net initiative. More information about BioModels Database can be found in the Frequently Asked Questions.





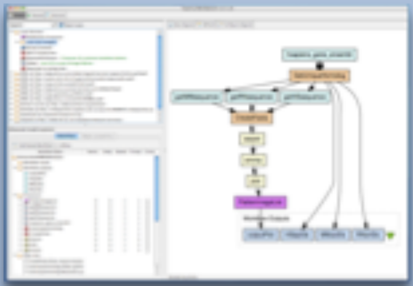


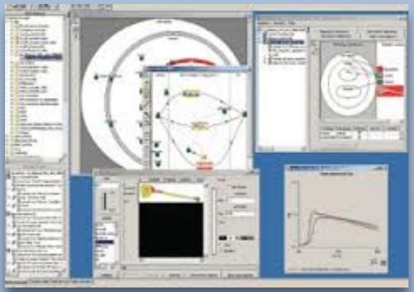
```
Ok
p = defn Jana_WolfGlycolysis

vol compartment;
var Glucose, fructose_1_6_bisphosphate, glyceraldehyde_3_phosphate, glycerate_3_phosphate,
       pyruvate, Acetyladehyde, External_acetaldehyde, ATP,
       ADP, NAD, NADH;
ext External_glucose, ethanol, Glycerol, Sink;

J0: $External_glucose -> Glucose; J0_inputFlux;
J1: Glucose + 2 ATP -> fructose_1_6_bisphosphate + 2 ADP; J1_k1*Glucose*ATP*(1/(1+pow(ATP/J1_Ki,J1_n)));
J2: fructose_1_6_bisphosphate -> glyceraldehyde_3_phosphate + glyceraldehyde_3_phosphate;
J2_J2_k*fructose_1_6_bisphosphate;
J3: glyceraldehyde_3_phosphate + NADH -> NAD + $Glycerol; J3_J3_k*glyceraldehyde_3_phosphate*NADH;
J4: glyceraldehyde_3_phosphate + ADP + NAD -> ATP + glycerate_3_phosphate + NADH;
(J4_kg*J4_kp*glyceraldehyde_3_phosphate*NAD*ADP-J4_ka*J4_kk*glycerate_3_phosphate*ATP*NADH)/(J4_ka*NADH+J4_kp*ADP);
J5: glycerate_3_phosphate + ADP -> ATP + pyruvate; J5_J5_k*glycerate_3_phosphate*ADP;
J6: pyruvate -> Acetyladehyde; J6_J6_k*pyruvate;
```



Welcome!

SABIO-RK is a curated database that contains information about biochemical react their kinetic rate equations with parameters and experimental conditions.



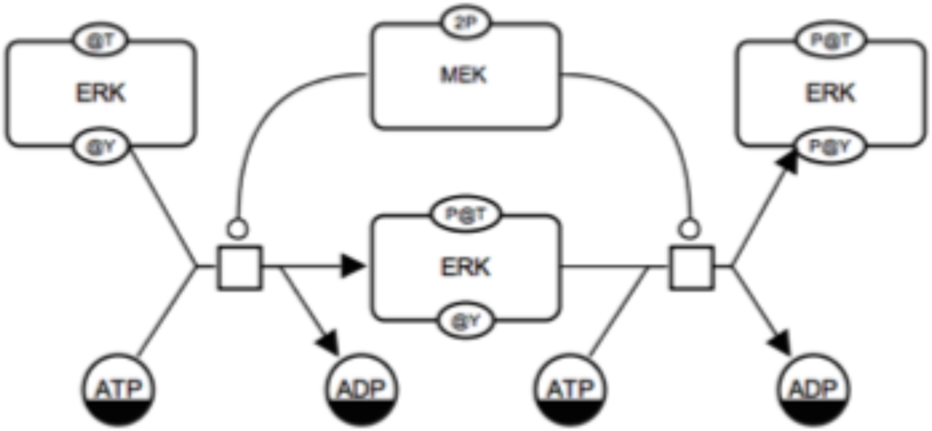


SBML = format for exchanging biological models between tools

Hucka M, Finney A, Sauro HM, *et al.*: **The systems biology markup language (SBML): a medium for representation and exchange of biochemical network models**. Bioinformatics (2003) 19(4): 524-531

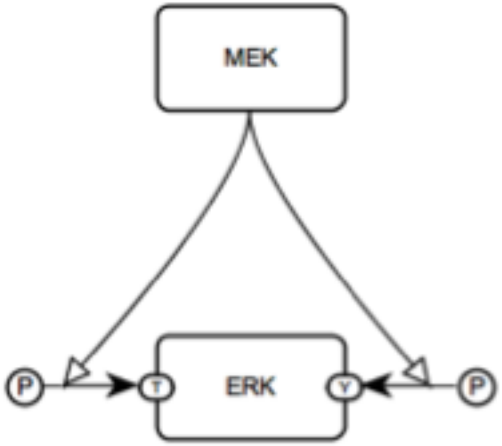
Systems Biology Graphical Notation: SBGN

Process Description maps



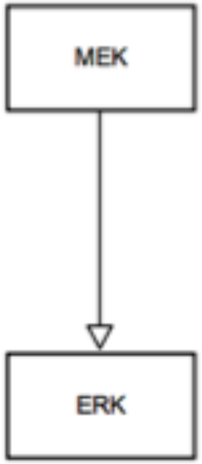
- Unambiguous
- Mechanistic
- Sequential
- Combinatorial explosion

Entity Relationships maps



- Unambiguous
- Mechanistic
- Non-Sequential

Activity Flow maps



- Ambiguous
- Conceptual
- Sequential

Le Novère N, Hucka M, Mi H, Moodie S, Schreiber F, Sorokin A, Demir E, Wegner K, Aladjem MI, Wimalaratne SM, Bergman FT, Gauges R, Ghazal P, Kawaji H, Li L, Matsuoka Y, Villéger A, Boyd SE, Calzone L, *et al.*
The Systems Biology Graphical Notation. Nature Biotechnology 27(8):735-41 (2009)

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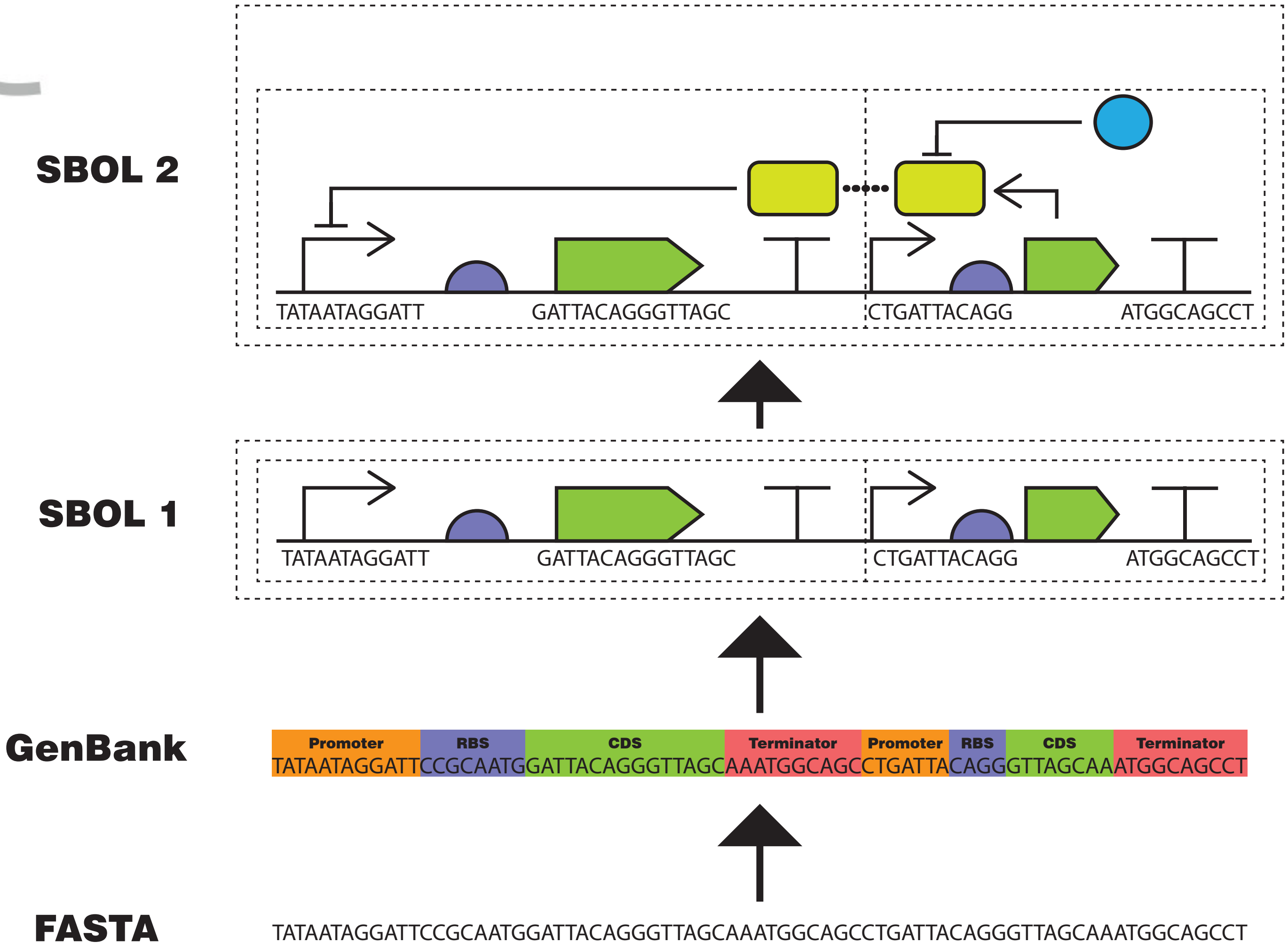
http://www.sbgn.org

SBOL



SBOL 2

TATAATAGGATT GATTACAGGGTTAGC CTGATTACAGG ATGGCAGCCT

SBOL 1

TATAATAGGATT GATTACAGGGTTAGC CTGATTACAGG ATGGCAGCCT

GenBank

Promoter	RBS	CDS	Terminator	Promoter	RBS	CDS	Terminator
TATAATAGGATT	CCGCAATG	GATTACAGGGTTAGC	AAATGGCAGC	CTGATTA	CAGG	GTTAGCAA	ATGGCAGCCT

FASTA

TATAATAGGATTCCGCAATGGATTACAGGGTTAGCAAATGGCAGCCTGATTACAGGGTTAGCAAATGGCAGCCT

Michal Galdzicki, Kevin P. Clancy, Ernst Oberortner, Matthew Pocock, Jacqueline Quinn, Cesar A. Rodriguez, Nicholas Roehner, Mandy L. Wilson, *et al.*: **The Synthetic Biology Open Language (SBOL) provides a community standard for communicating designs in synthetic biology**. Nature Biotechnology 32, 545-550 (2014)

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http://sbolstandard.org

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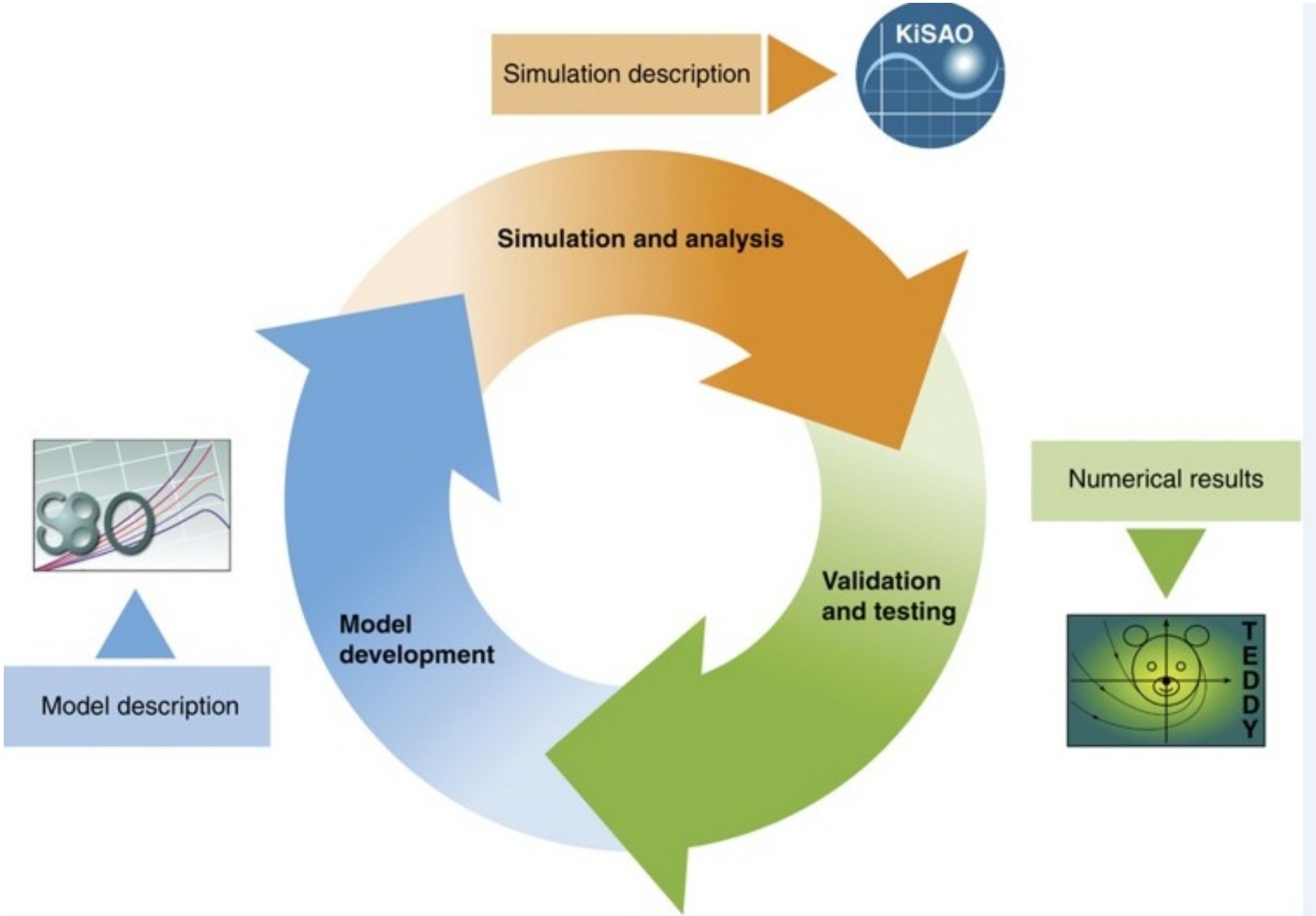
Terminologies, Ontologies and Controlled Vocabulary



Courtot M, Juty N, Knüpfer C, Waltemath D, Zhukova A, Dräger A, Dumontier M, Finney A, Golebiewski M, Hastings J, Hoops S, Keating S, Kell DB, Kerrien S, Lawson J, Lister A, Lu J, Machne R, Mendes P, Pocock M, Rodriguez N, Villeger A, Wilkinson DJ, Wimalaratne S, Laibe C, Hucka M, Le Novère N: Controlled vocabularies and semantics in systems biology. Mol Syst Biol. 2011 Oct 25;7:543

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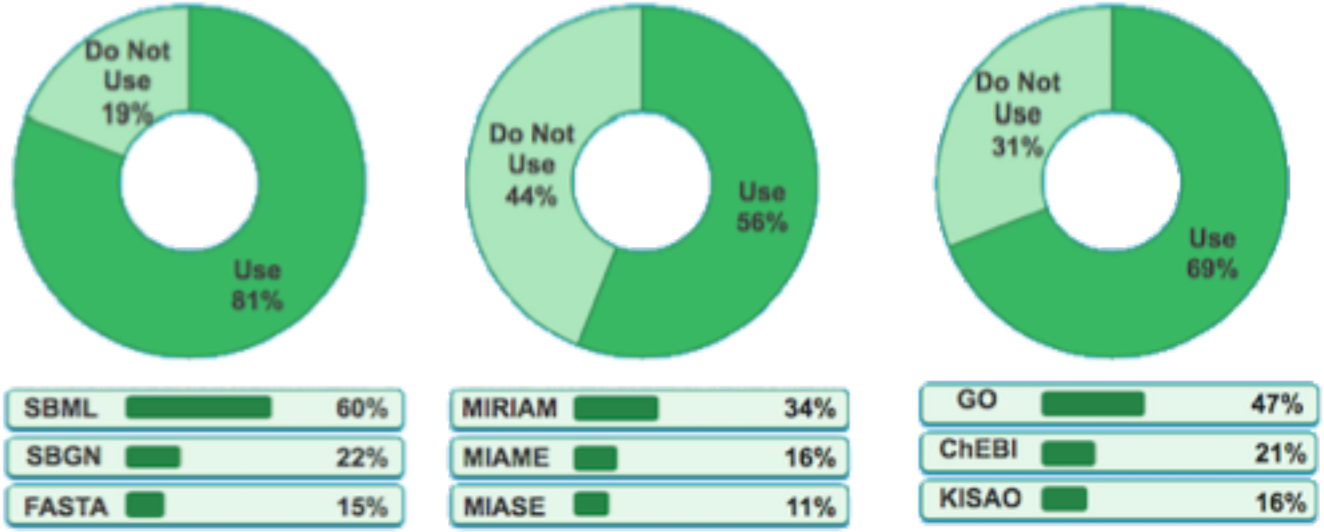
Researchers do not always use data, metadata or model standards

Format

Metadata

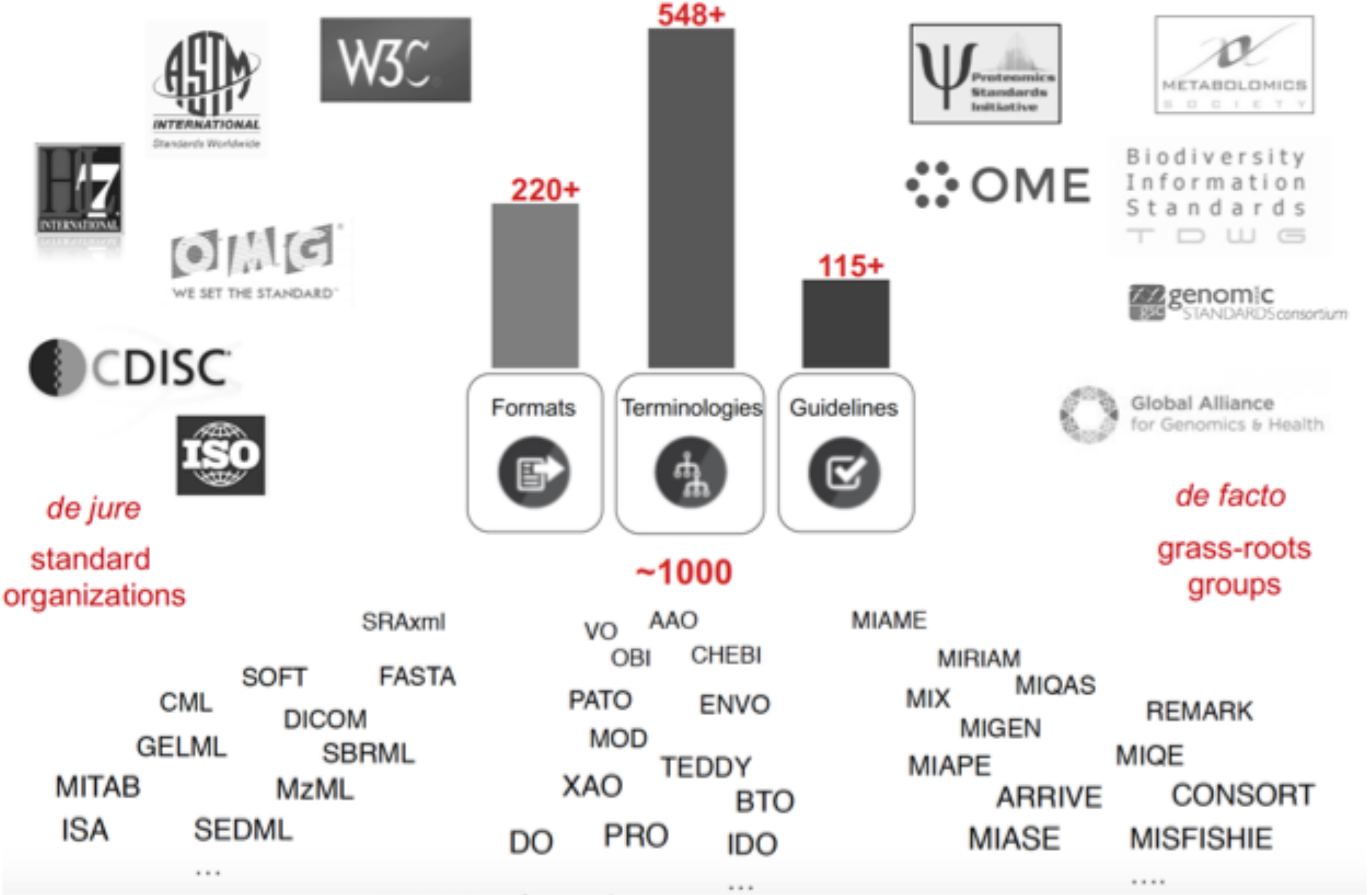
Ontologies



*top three most popular

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

Community (de-facto) standards in life sciences



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FAIRsharing.org standards, databases, policies

https://fairsharing.org

Source: Susanna-Assunta Sansone (University of Oxford, UK)

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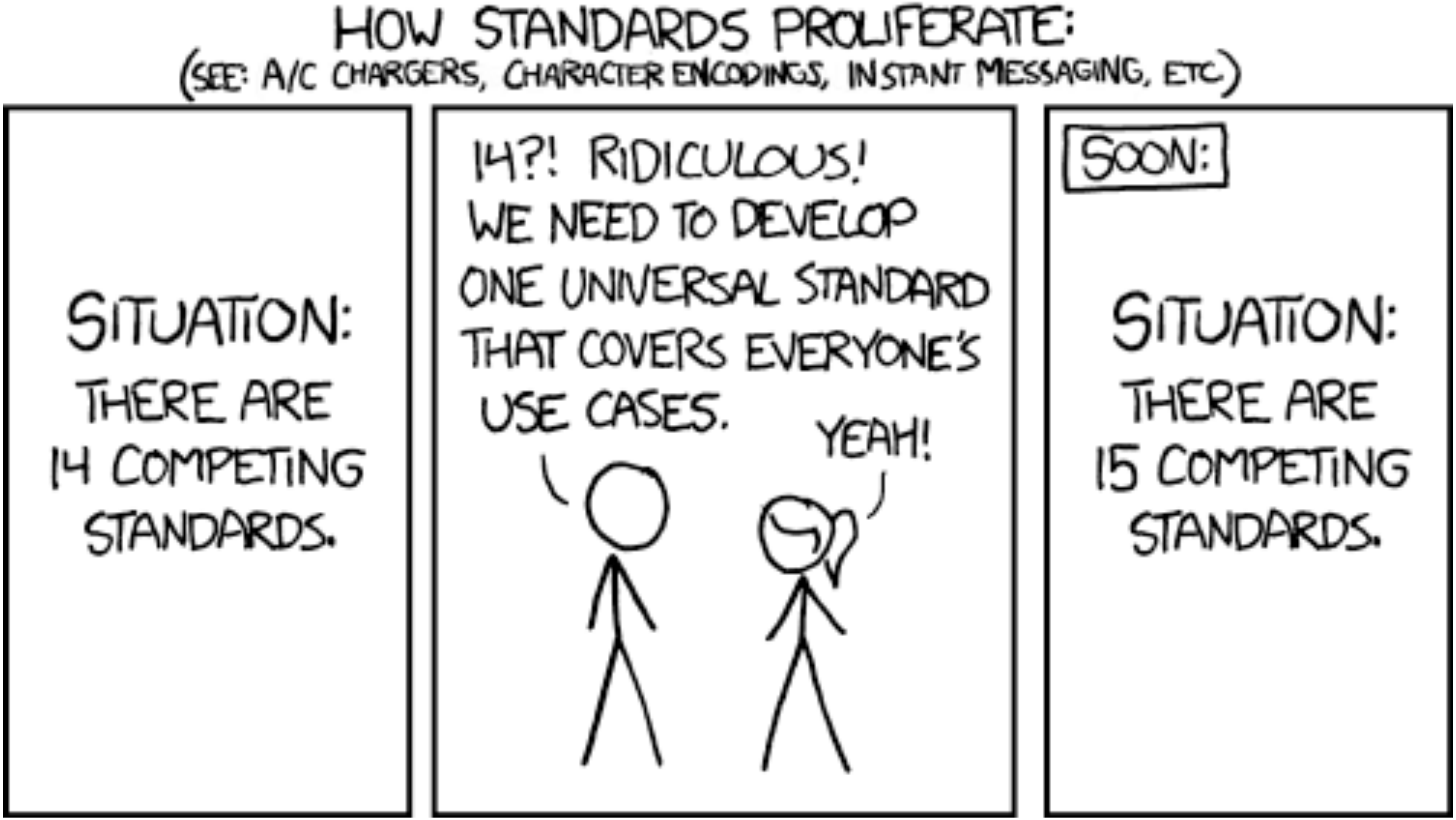
So many standards...



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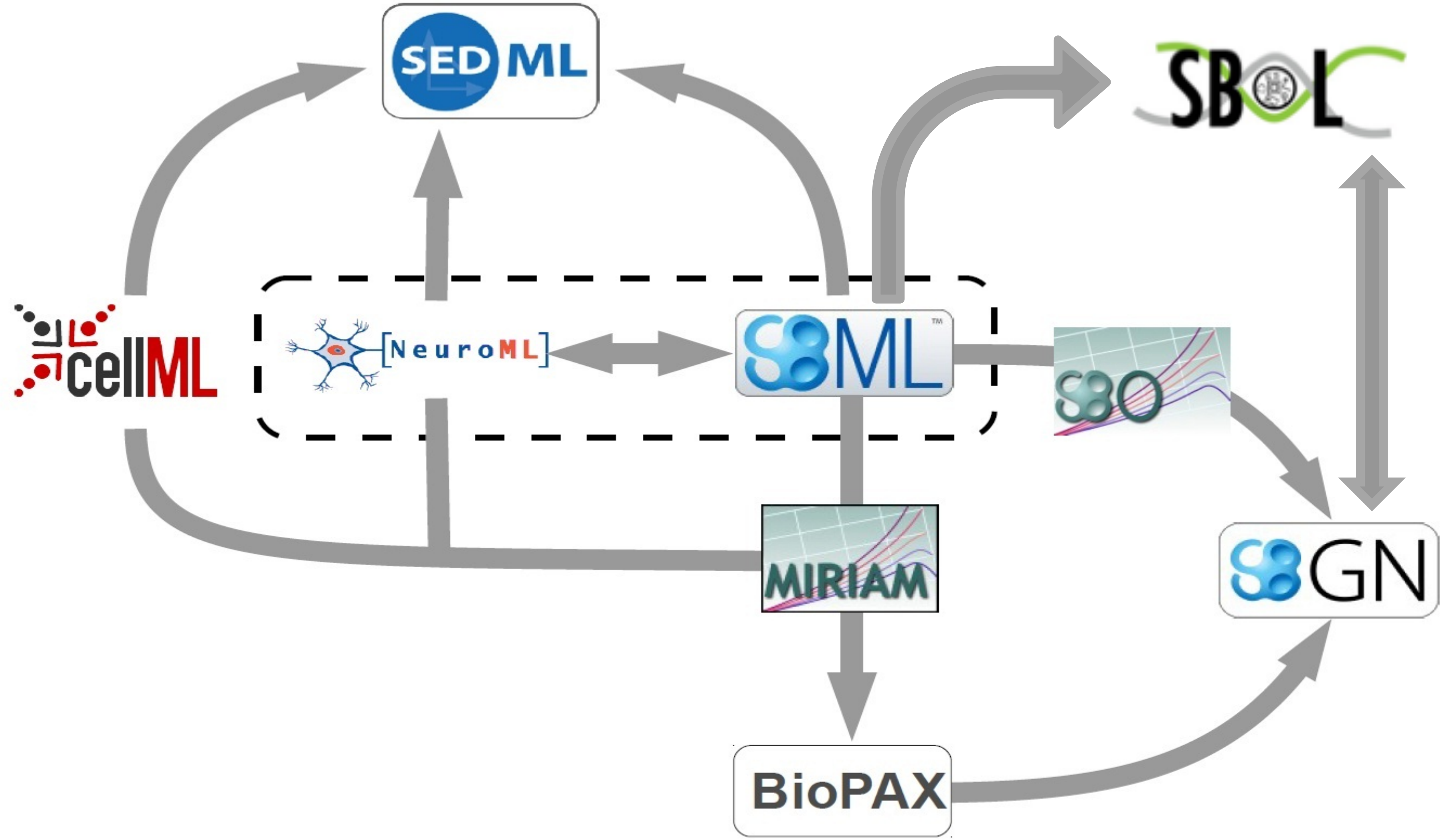
Interoperability of Modelling Standards



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Harmonized standard formats ensure the interoperability of data & models

Example: Great Baltimore fire of 1904

Individual fire hydrants depending on region with 600 variations of hose couplings

→ Need for interoperability of formats

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ERASysAPP ERA-Net for Applied Systems Biology

LiSyM

Coordination of standard development in systems biology

the combine
computational modeling in biology network

http://co.mbine.org/

The "WorldWide Web consortium" of modelling in biology

Interoperable Standards
For modelling in biology

Hucka M, Nickerson DP, Bader GD, Bergmann FT, Cooper J, Demir E, Garny A, Golebiewski M, Myers CJ, Schreiber F, Waltemath D, Le Novère N:
Promoting Coordinated Development of Community-Based Information Standards for Modeling in Biology: The COMBINE Initiative
Front Bioeng Biotechnol. (2015) 3:19. doi: 10.3389/fbioe.2015.00019

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Overview of the COMBINE standards

Core Standards

Standards for Knowledge Representation

BioPAX

SBOL

Standards for Visual Representation

SBGN

SBOL VISUAL

Standards for Models and their Analyses

SBML

CellML

NeuroML

SED-ML

Associated Standards

Used by core standards

Projects

Infrastructure

BioModels.net qualifiers

Controlled Vocabularies

SBO

KiSAO

adapted from:
Schreiber F, Bader GD, Gleeson P, Golebiewski M, Hucka M, Le Novère N, Myers C, Nickerson D, Sommer B, Walthemath D:
Specifications of Standards in Systems and Synthetic Biology: Status and Developments in 2016
J Integr Bioinform. (2016) 13:289. doi: 10.2390/biecoll-jib-2016-289

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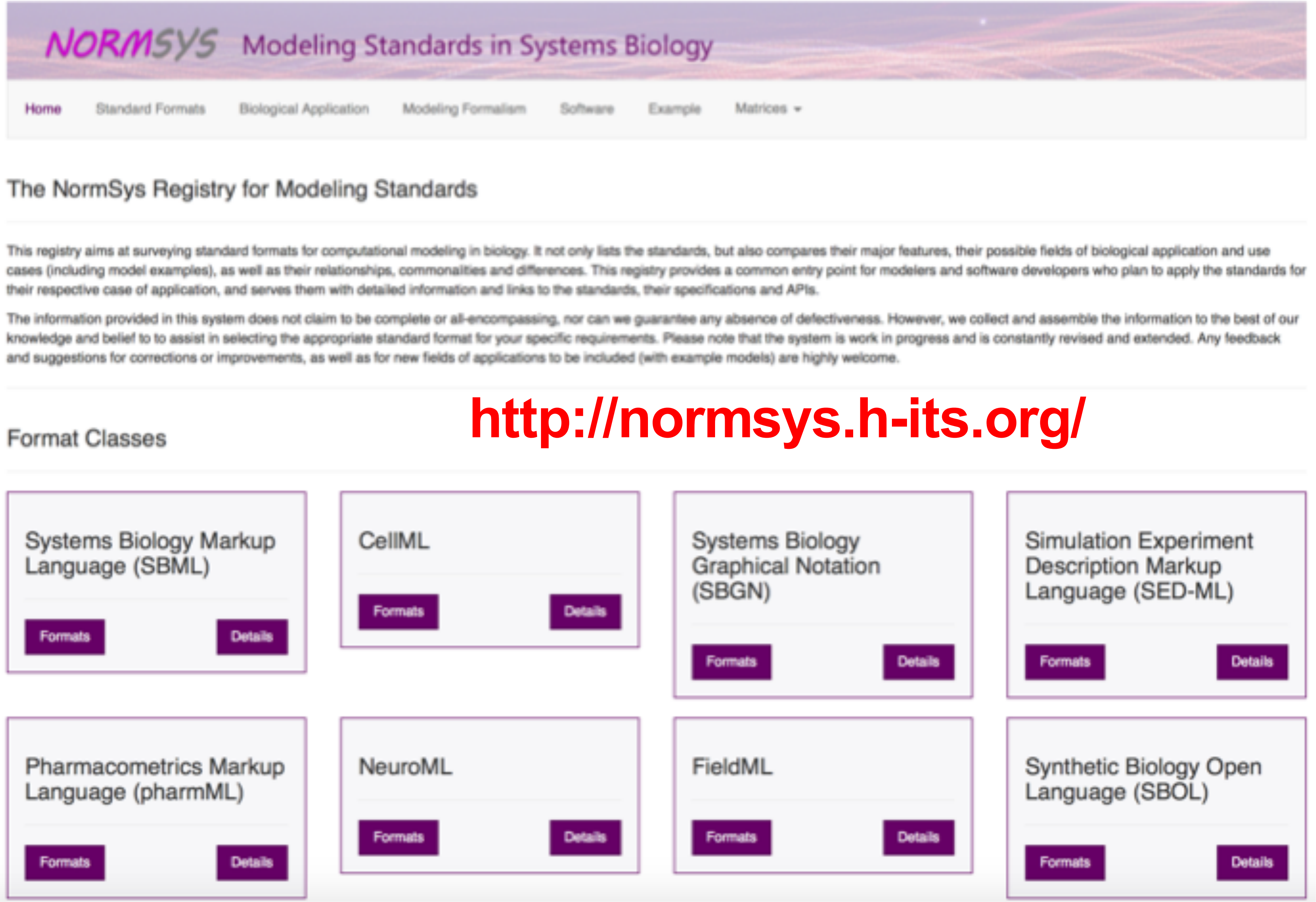

The NormSys Registry for Modeling Standards

This registry aims at surveying standard formats for computational modeling in biology. It not only lists the standards, but also compares their major features, their possible fields of biological application and use cases (including model examples), as well as their relationships, commonalities and differences. This registry provides a common entry point for modelers and software developers who plan to apply the standards for their respective case of application, and serves them with detailed information and links to the standards, their specifications and APIs.

The information provided in this system does not claim to be complete or all-encompassing, nor can we guarantee any absence of defectiveness. However, we collect and assemble the information to the best of our knowledge and belief to to assist in selecting the appropriate standard format for your specific requirements. Please note that the system is work in progress and is constantly revised and extended. Any feedback and suggestions for corrections or improvements, as well as for new fields of applications to be included (with example models) are highly welcome.

http://normsys.h-its.org/

Format Classes

- Systems Biology Markup Language (SBML)
- CellML
- Systems Biology Graphical Notation (SBGN)
- Simulation Experiment Description Markup Language (SED-ML)
- Pharmacometrics Markup Language (pharmML)
- NeuroML
- FieldML
- Synthetic Biology Open Language (SBOL)

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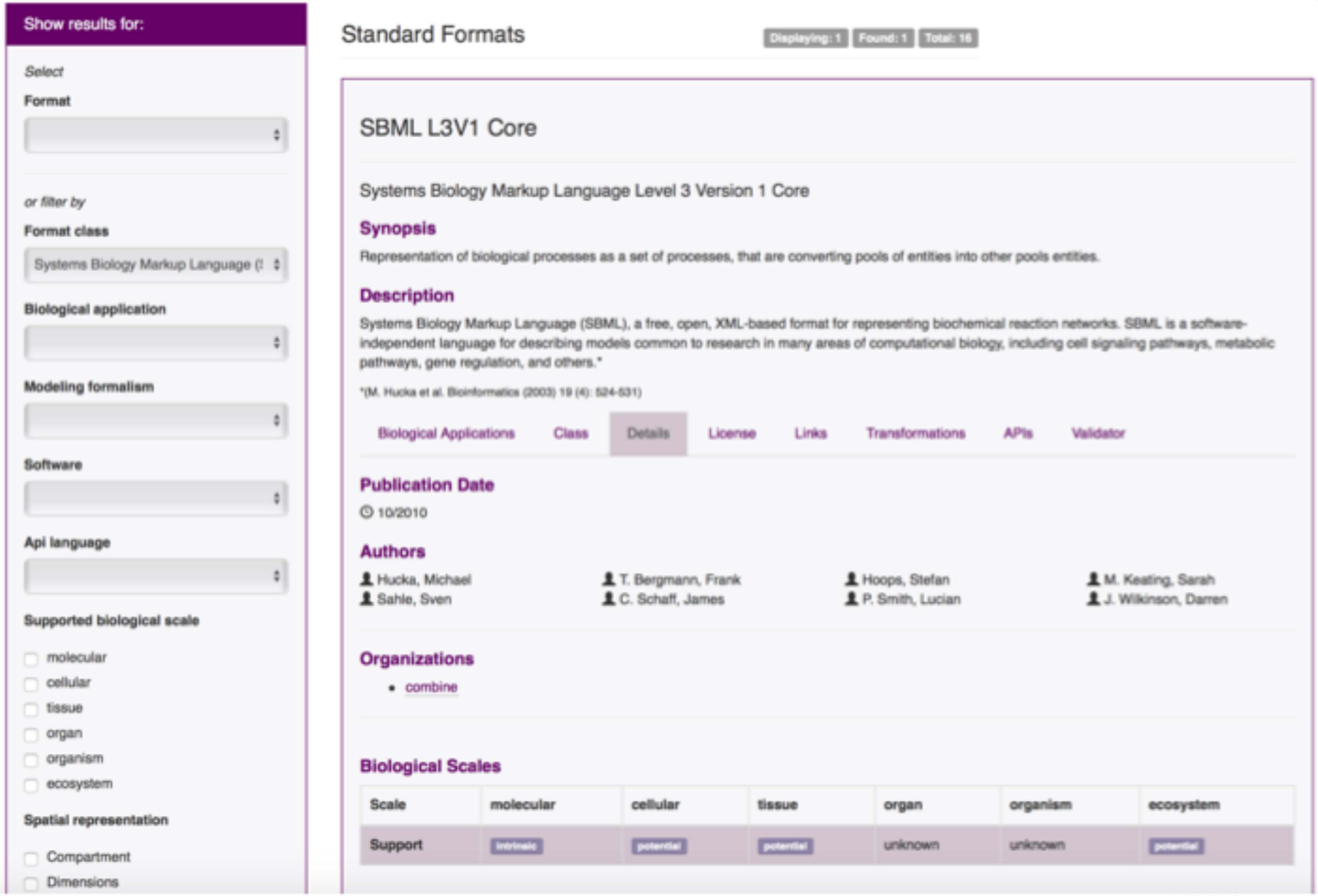

Format class: Systems Biology Markup Language (S

Supported biological scale:
☐ molecular
☐ cellular
☐ tissue
☐ organ
☐ organism
☐ ecosystem

Spatial representation:
☐ Compartment
☐ Dimensions

Standard Formats

SBML L3V1 Core

Systems Biology Markup Language Level 3 Version 1 Core

Synopsis

Representation of biological processes as a set of processes, that are converting pools of entities into other pools entities.

Description

Systems Biology Markup Language (SBML), a free, open, XML-based format for representing biochemical reaction networks. SBML is a software-independent language for describing models common to research in many areas of computational biology, including cell signaling pathways, metabolic pathways, gene regulation, and others.*

*(M. Hucka et al. Bioinformatics (2003) 19 (4): 524-531)

Publication Date

10/2010

Authors

Hucka, Michael	T. Bergmann, Frank	Hoops, Stefan	M. Keating, Sarah
Sahle, Sven	C. Schaff, James	P. Smith, Lucian	J. Wilkinson, Darren

Organizations

- combine

Biological Scales

Scale	molecular	cellular	tissue	organ	organism	ecosystem
Support	intrinsic	potential	potential	unknown	unknown	potential

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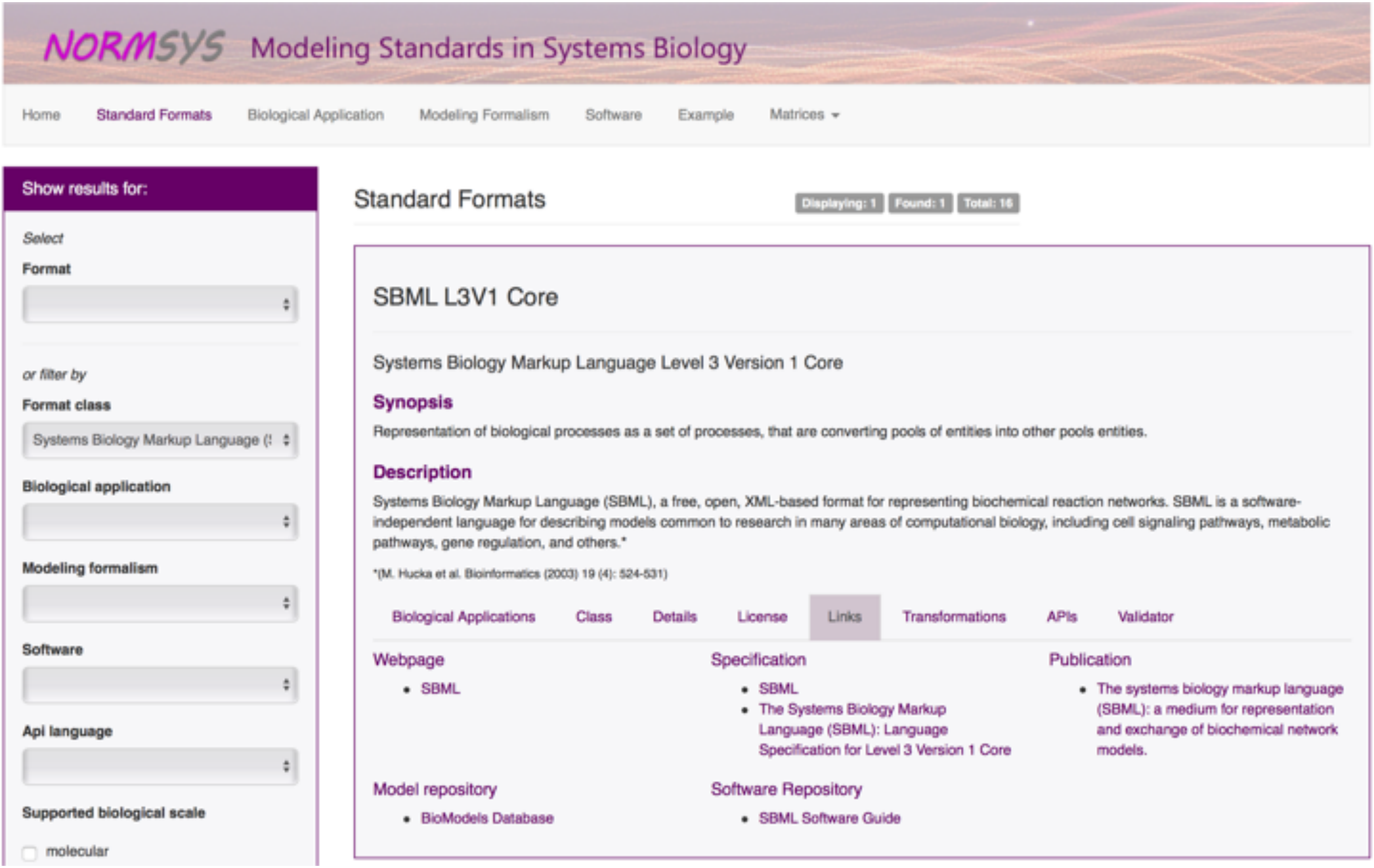

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*(M. Hucka et al. Bioinformatics (2003) 19 (4): 524-531)

Webpage

- SBML

Specification

- SBML
- The Systems Biology Markup Language (SBML): Language Specification for Level 3 Version 1 Core

Publication

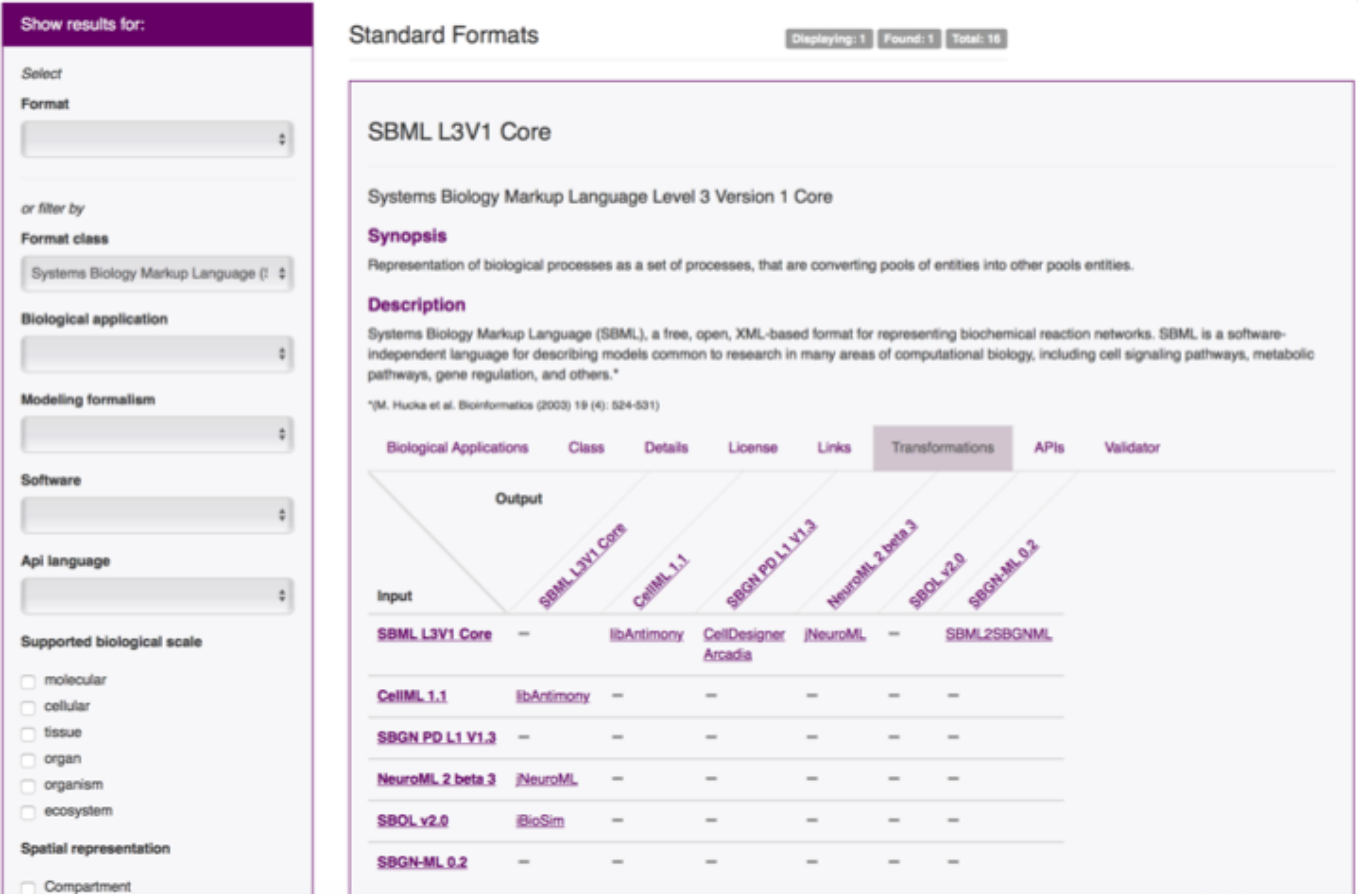
- The systems biology markup language (SBML): a medium for representation and exchange of biochemical network models.

Model repository

- BioModels Database

Software Repository

- SBML Software Guide



Show results for:

Select

Format

or filter by

Format class: Systems Biology Markup Language (

Biological application

Modeling formalism

Software

Api language

Supported biological scale

☐ molecular
☐ cellular
☐ tissue
☐ organ
☐ organism
☐ ecosystem

Spatial representation

☐ Compartment

Standard Formats

Displaying: 1 Found: 1 Total: 16

SBML L3V1 Core

Systems Biology Markup Language Level 3 Version 1 Core

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*(M. Hucka et al. Bioinformatics (2003) 19 (4): 524-531)

Input \ Output	SBML L3V1 Core	CellML 1.1	SBGN PD L1 V1.3	NeuroML 2 beta 3	SBOL v2.0	SBGN-ML 0.2
SBML L3V1 Core	–	libAntimony	CellDesigner Arcadia	jNeuroML	–	SBML2SBGNML
CellML 1.1	libAntimony	–	–	–	–	–
SBGN PD L1 V1.3	–	–	–	–	–	–
NeuroML 2 beta 3	jNeuroML	–	–	–	–	–
SBOL v2.0	iBioSim	–	–	–	–	–
SBGN-ML 0.2	–	–	–	–	–	–

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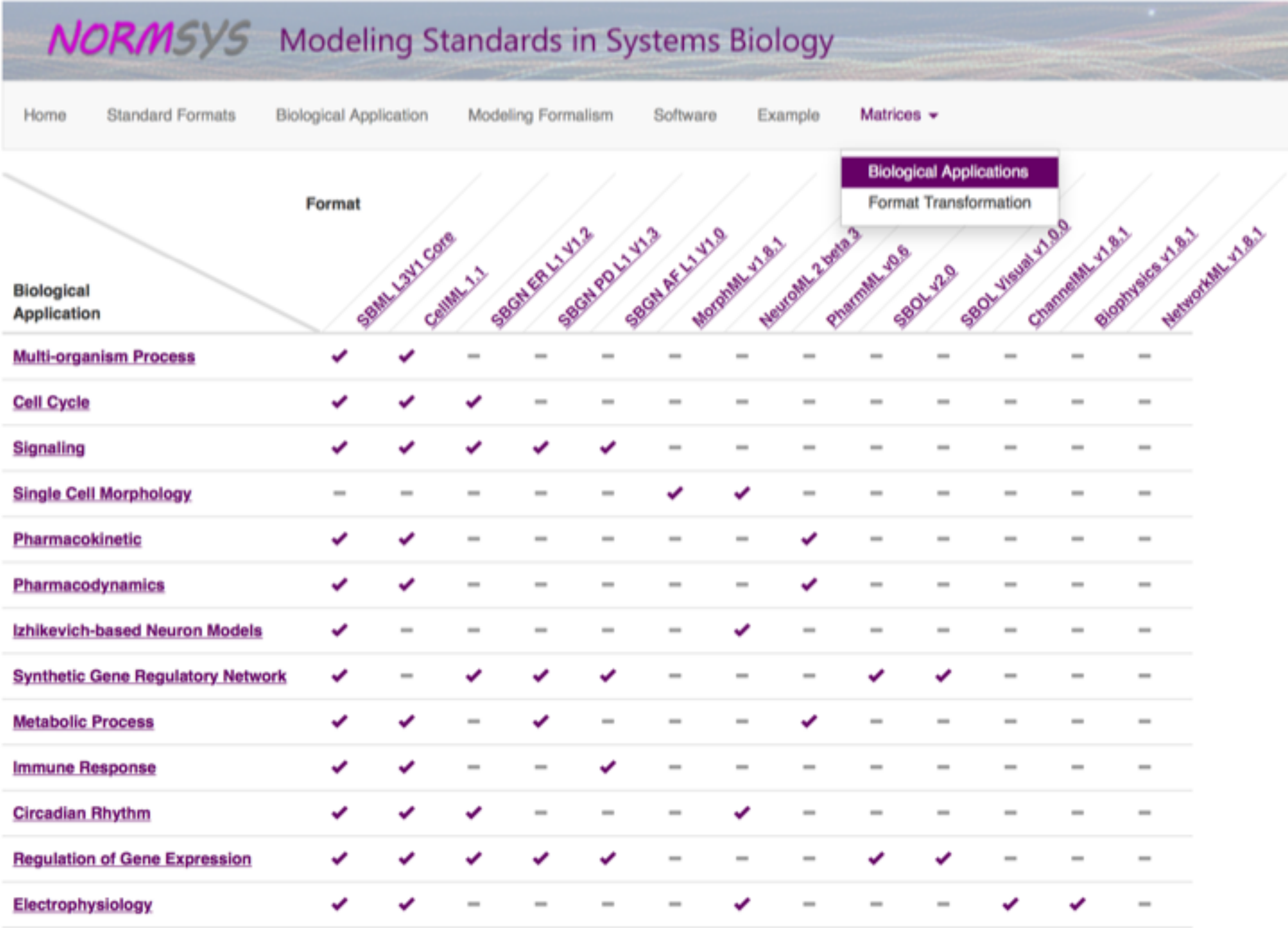
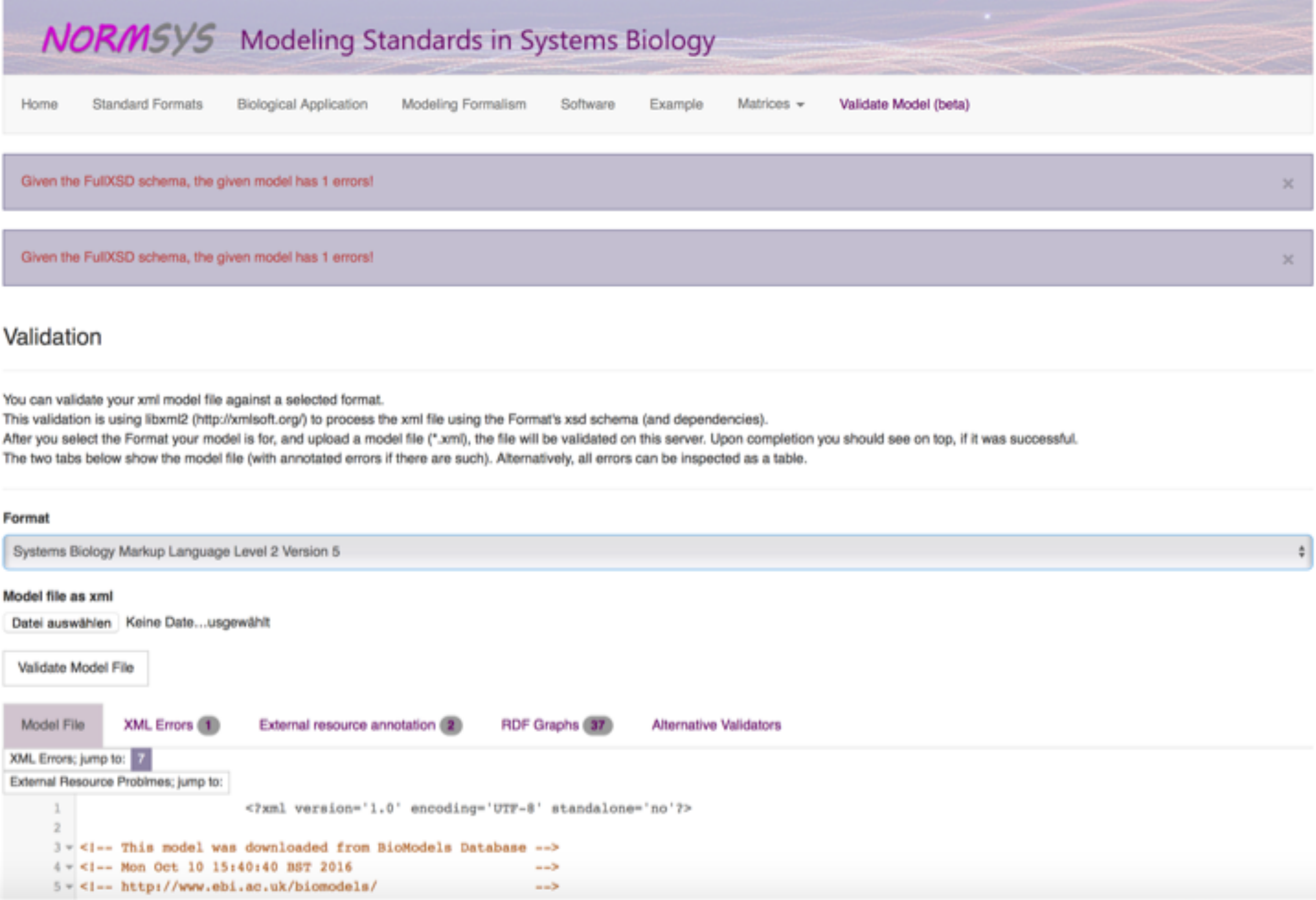


Biological Application / Format	SBML L3V1 Core	CellML 1.1	SBGN ER L1 V1.2	SBGN PD L1 V1.3	SBGN AF L1 V1.0	MorphML v1.8.1	NeuroML 2 beta 3	PharmML v0.6	SBOL v2.0	SBOL Visual v1.0.0	ChannelML v1.8.1	Biophysics v1.8.1	NetworkML v1.8.1
Multi-organism Process	✓	✓	—	—	—	—	—	—	—	—	—	—	—
Cell Cycle	✓	✓	✓	—	—	—	—	—	—	—	—	—	—
Signaling	✓	✓	✓	✓	✓	—	—	—	—	—	—	—	—
Single Cell Morphology	—	—	—	—	—	✓	✓	—	—	—	—	—	—
Pharmacokinetic	✓	✓	—	—	—	—	—	✓	—	—	—	—	—
Pharmacodynamics	✓	✓	—	—	—	—	—	✓	—	—	—	—	—
Izhikevich-based Neuron Models	✓	—	—	—	—	—	✓	—	—	—	—	—	—
Synthetic Gene Regulatory Network	✓	—	✓	✓	✓	—	—	—	✓	✓	—	—	—
Metabolic Process	✓	✓	—	✓	—	—	—	✓	—	—	—	—	—
Immune Response	✓	✓	—	—	✓	—	—	—	—	—	—	—	—
Circadian Rhythm	✓	✓	✓	—	—	—	✓	—	—	—	—	—	—
Regulation of Gene Expression	✓	✓	✓	✓	✓	—	—	—	✓	✓	—	—	—
Electrophysiology	✓	✓	—	—	—	—	✓	—	—	—	✓	✓	—



Given the FullXSD schema, the given model has 1 errors!

Given the FullXSD schema, the given model has 1 errors!

Validation

You can validate your xml model file against a selected format.
This validation is using libxml2 (http://xmlsoft.org/) to process the xml file using the Format's xsd schema (and dependencies).
After you select the Format your model is for, and upload a model file (*.xml), the file will be validated on this server. Upon completion you should see on top, if it was successful.
The two tabs below show the model file (with annotated errors if there are such). Alternatively, all errors can be inspected as a table.

Format

Systems Biology Markup Language Level 2 Version 5

Model file as xml

Datei auswählen Keine Date...usgewählt

```
                  <?xml version='1.0' encoding='UTF-8' standalone='no'?>

<!-- This model was downloaded from BioModels Database -->
<!-- Mon Oct 10 15:40:40 BST 2016                      -->
<!-- http://www.ebi.ac.uk/biomodels/                   -->
```

NORMSYS

Supported by:
Federal Ministry for Economic Affairs and Energy

https://normsys.h-its.org/validate

HITS

FAIRDOM

FAIRDOM data management: Share your data FAIR

www.fair-dom.org

Findable

Accessible

Interoperable

Reusable

Data

Operating procedures

Models

Heidelberg Institute for Theoretical Studies

HITS

MANCHESTER 1824

The University of Manchester

UNIVERSITEIT·STELLENBOSCH·UNIVERSITY

jou kennisvennoot·your knowledge partner

HITS

de.NBI

German Network for Bioinformatics Infrastructure

ERASysAPP

ERA-Net for Applied Systems Biology

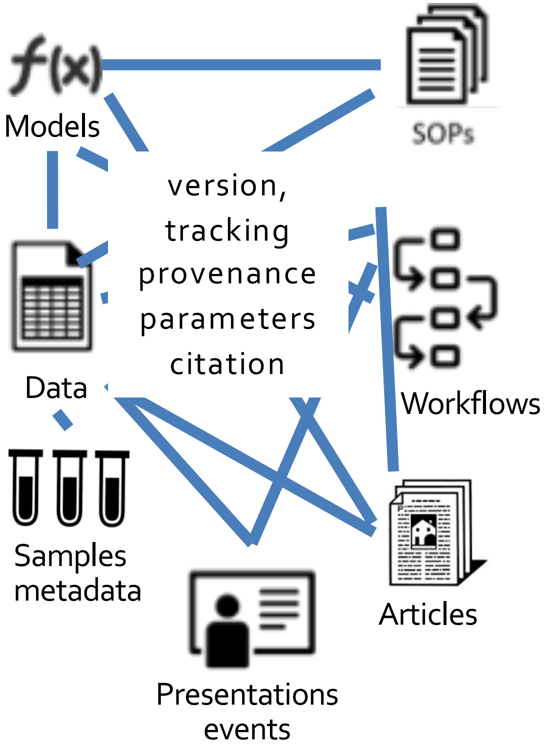
LiSyM

Liver Systems Medicine

Sponsored by the Federal Ministry of Education and Research

FAIRDOM pillars

- Community Actions
- Project Stewardship Services
- A Central Public Hub for Projects
- Project Specific Installations
- Software Platform + Tools



Models

SOPs

Data

Workflows

Samples
metadata

Articles

Presentations
events

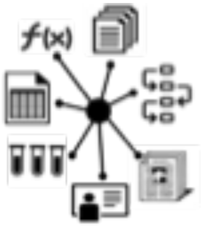
version,
tracking
provenance
parameters
citation

Metadata People Processes

FAIRDOM asset management

an ecosystem of resources

Sharing



Organisation

Front end

Projects Hub

Entry Point

Web-based portal
Project spaces
Metadata catalogue
Yellow pages
Results repository
Collaboration
Archives Gateway

Back end

Onsite storage & analytics

On site
Tracking
Pipelines
LIMS, Instruments
Large data
Samples
Auto-archiving

openBIS

NeLS
Norwegian e-Infratructure for Life Sciences

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ERASysAPP
ERA-Net for Applied Systems Biology

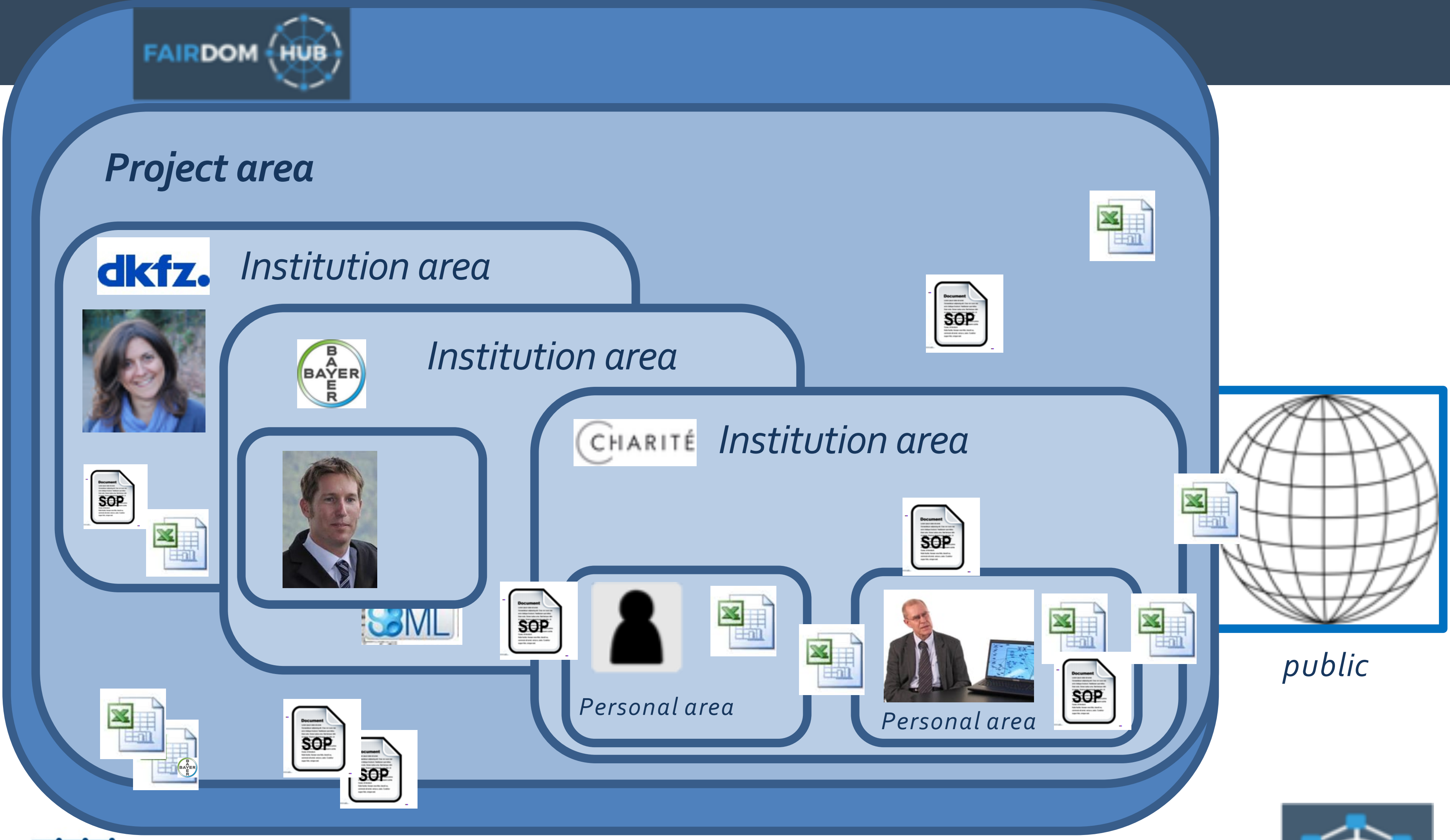
LiSyM

SEEK as a local (project-specific) instance or as FAIRDOMHub in the cloud

Service hosted at HITS
Institutional Guarantee at least until 2029

Wolstencroft, Owen, Krebs, Nguyen, Stanford, Golebiewski, et al. (2015):
SEEK: a systems biology data and model management platform,
BMC Systems Biology, 9:33 (doi: 10.1186/s12918-015-0174-y)

Self-managed sharing spaces



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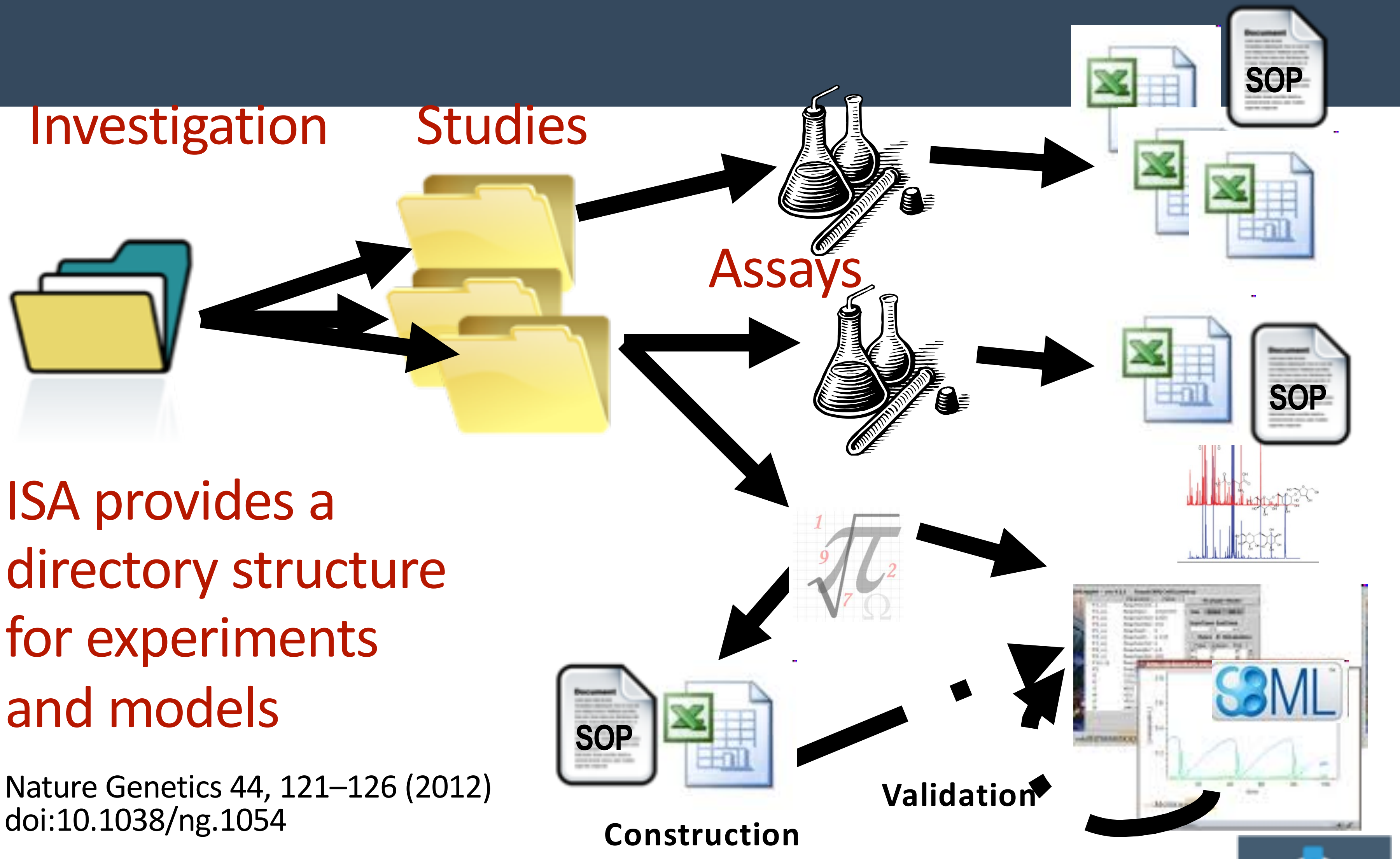
Federal Ministry of Education and Research

ISA: Organising and linking assets

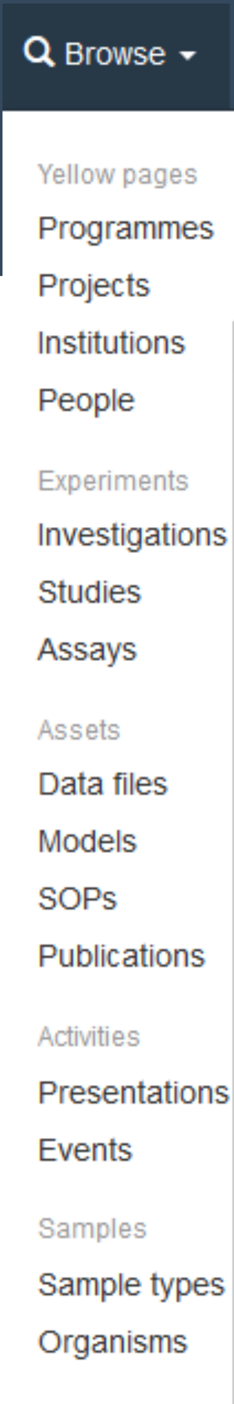


ISA provides a directory structure for experiments and models

Nature Genetics 44, 121–126 (2012)
doi:10.1038/ng.1054

HITS MANCHESTER 1824 The University of Manchester de.NBI ERASysAPP LiSyM

Cross-relating experiments & models: Context of investigations/studies



Browse

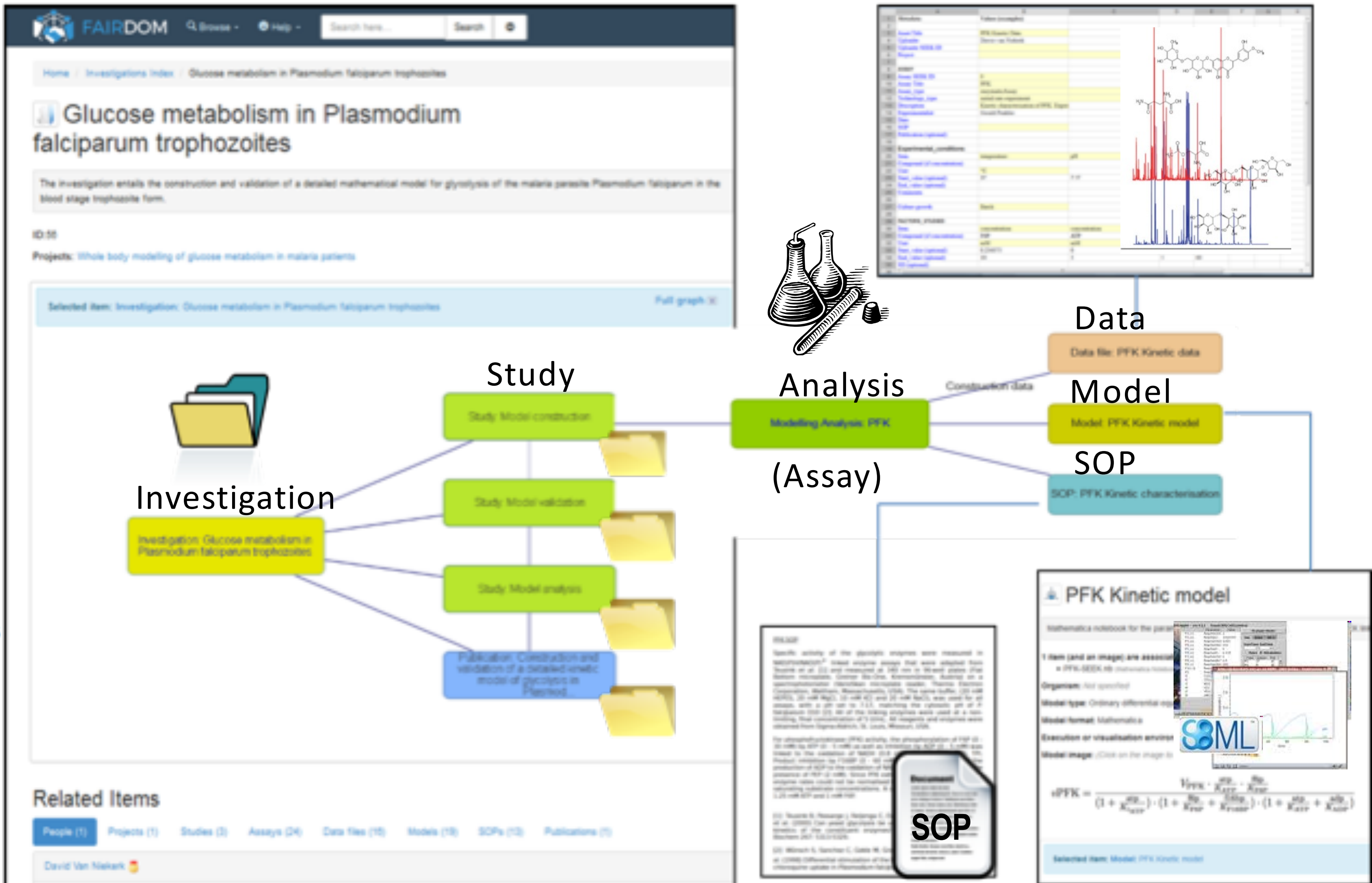
Yellow pages
- Programmes
- Projects
- Institutions
- People

Experiments
- Investigations
- Studies
- Assays

Assets
- Data files
- Models
- SOPs
- Publications

Activities
- Presentations
- Events

Samples
- Sample types
- Organisms



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:58

Projects: Whole body modelling of glucose metabolism in malaria patients

Selected item: Investigation: Glucose metabolism in Plasmodium falciparum trophozoites

Investigation

Investigation: Glucose metabolism in Plasmodium falciparum trophozoites

Study

Study: Model construction

Study: Model validation

Study: Model analysis

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

Analysis

Modelling Analysis: PFK

(Assay)

Construction data

Data

Data file: PFK Kinetic data

Model

Model: PFK Kinetic model

SOP

SOP: PFK Kinetic characterisation

Related Items

David Van Niekerk

PFK Kinetic model

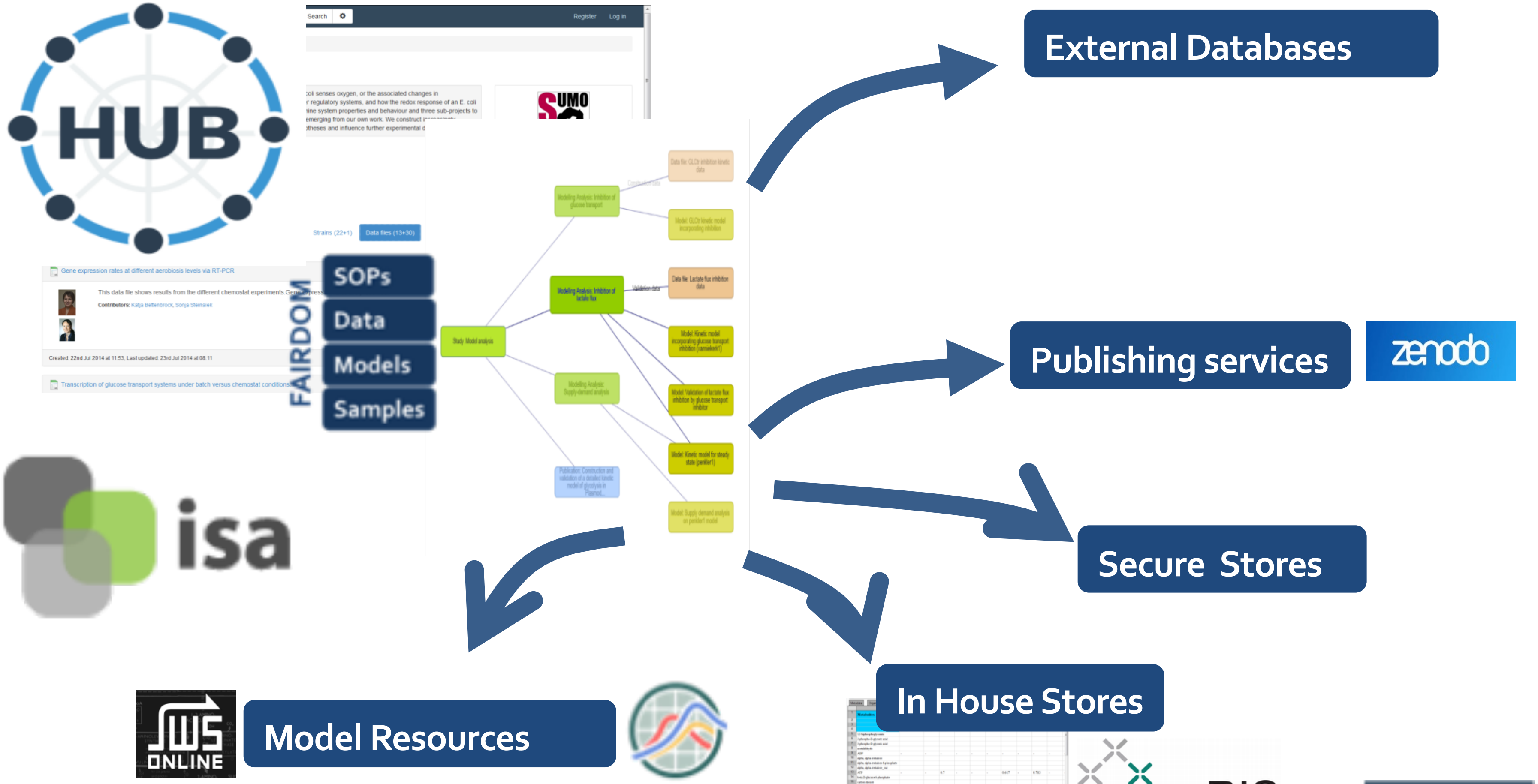
Organism: Not specified

Model type: Ordinary differential equations

Model format: Mathematica

Selected item: Model: PFK Kinetic model

Store & catalogue - Aggregation across repositories



Search | Register | Log in

…coli senses oxygen, or the associated changes in …r regulatory systems, and how the redox response of an E. coli …ine system properties and behaviour and three sub-projects to …emerging from our own work. We construct … …otheses and influence further experimental …

Strains (22+1) | Data files (13+30)

Gene expression rates at different aerobiosis levels via RT-PCR

This data file shows results from the different chemostat experiments. Gene express…

Contributors: Katja Bettenbrock, Sonja Steinsiek

Created: 22nd Jul 2014 at 11:53, Last updated: 23rd Jul 2014 at 08:11

Transcription of glucose transport systems under batch versus chemostat conditions

External Databases

Publishing services

Secure Stores

In House Stores

Model Resources

JWS ONLINE

openBIS Biology Information System

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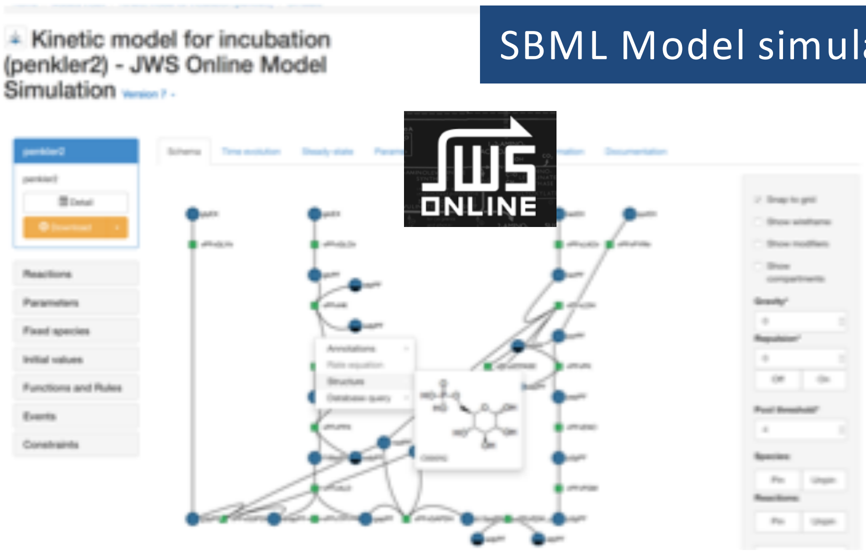
ERASysAPP ERA-Net for Applied Systems Biology

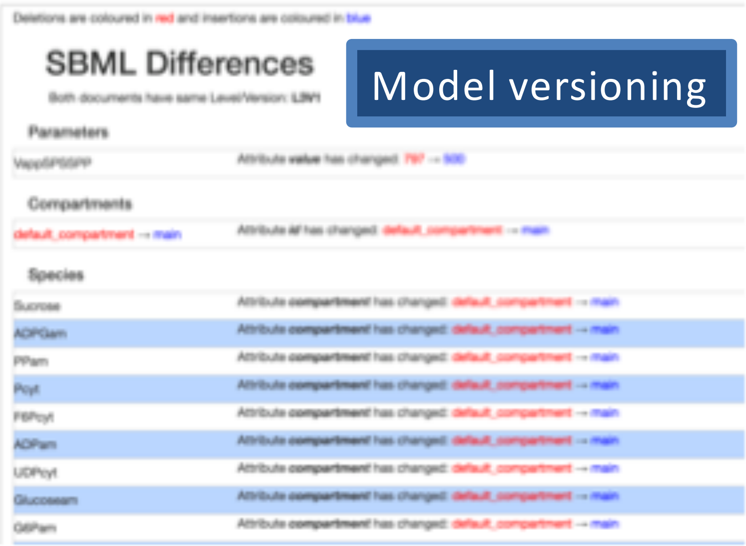
LiSyM

FAIRDOM modelling support



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

Parameters

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

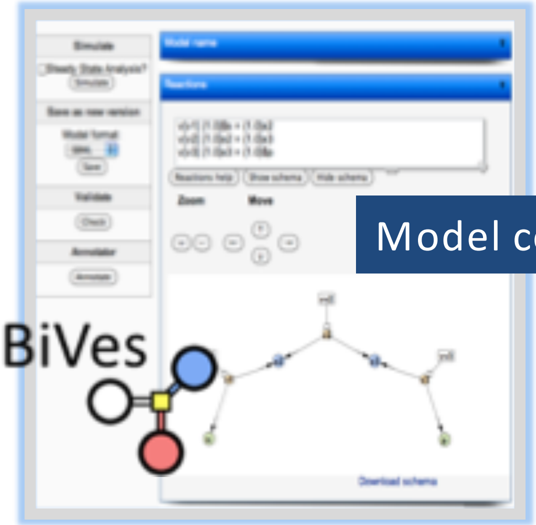
Compartments

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

Species

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

Model versioning

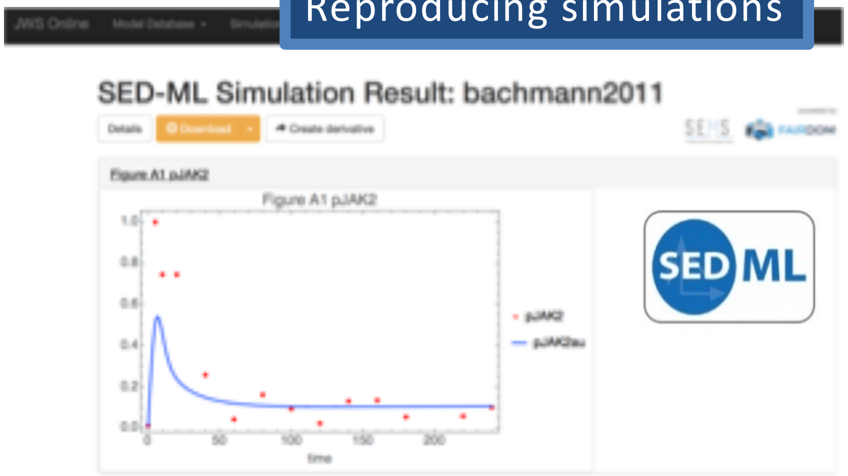


Model comparison

BiVes

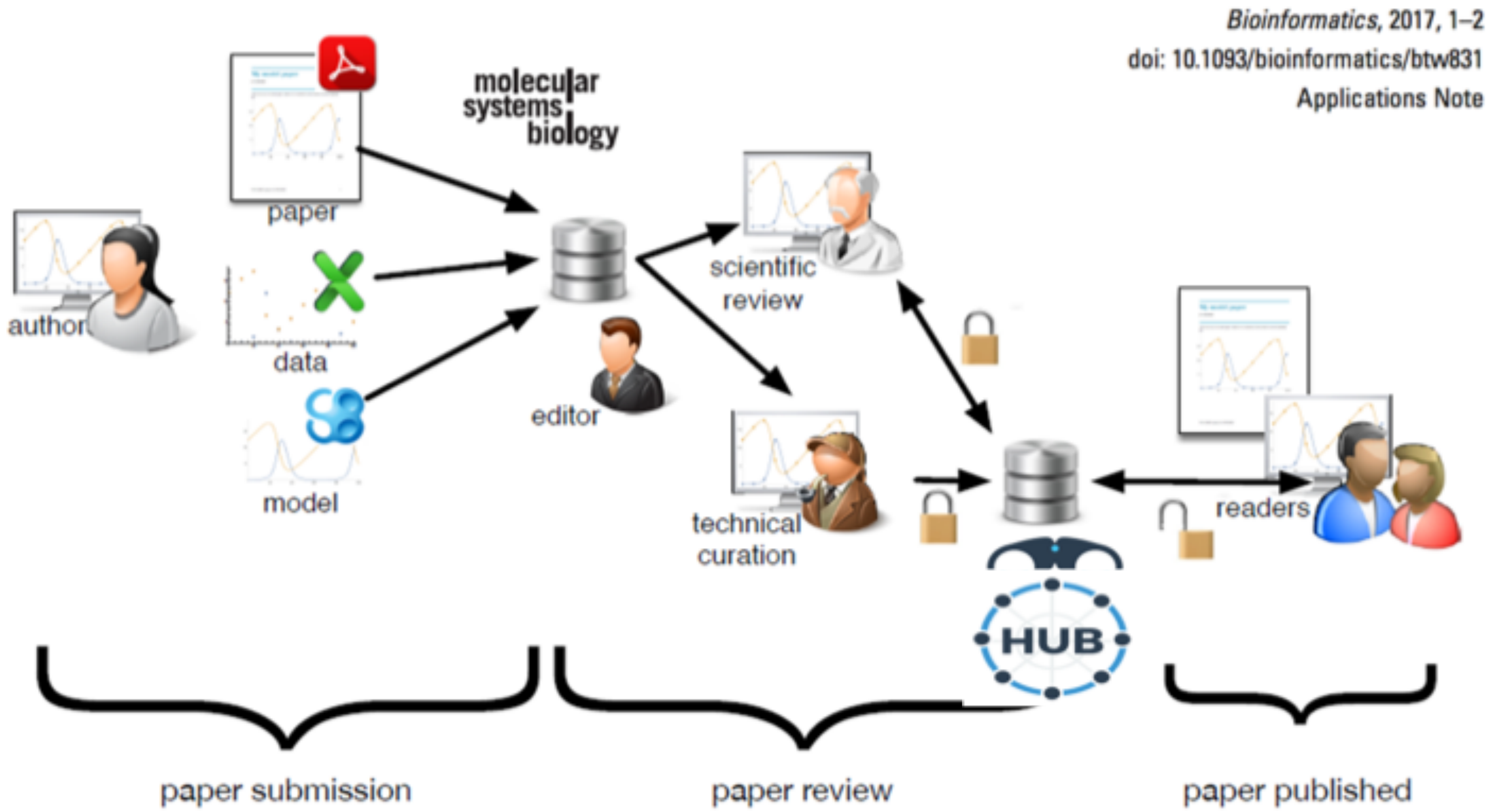
[Jacky Snoep, Dagmar Waltemath, Martin Peters, Martin Scharm]

Reproducing simulations



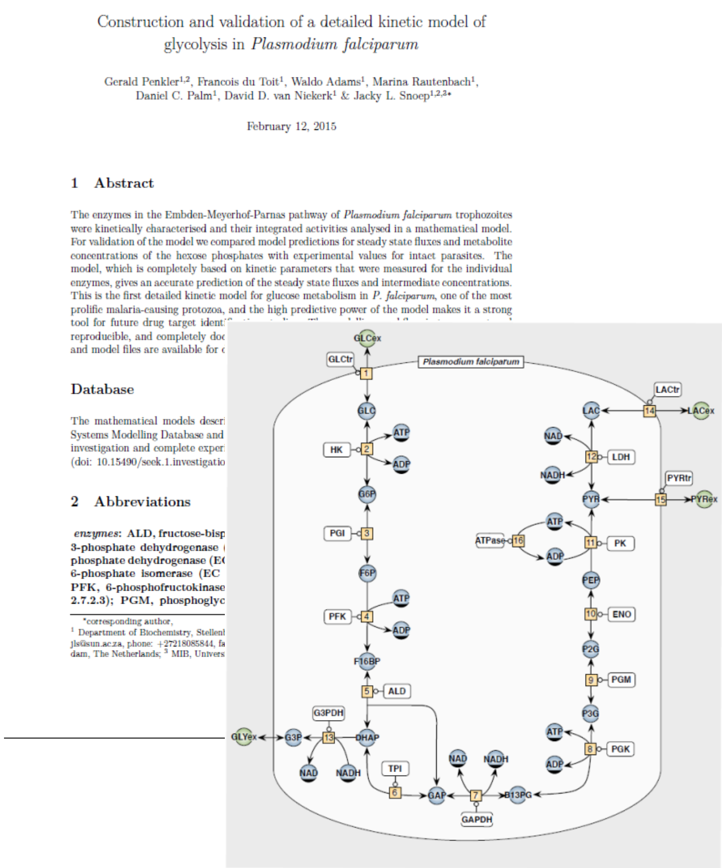
SED-ML Simulation Result: bachmann2011

Model curation. Reproducible Figures



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

FAIR Publishing support



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

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

February 12, 2015

1 Abstract

The enzymes in the Embden-Meyerhof-Parnas pathway of *Plasmodium falciparum* trophozoites were kinetically characterised and their integrated activities analysed 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 identi
reproducible, and completely doc
and model files are available for c

Database

The mathematical models descri
Systems Modelling Database and
investigation and complete experi
(doi: 10.15490/seek.1.investigatio

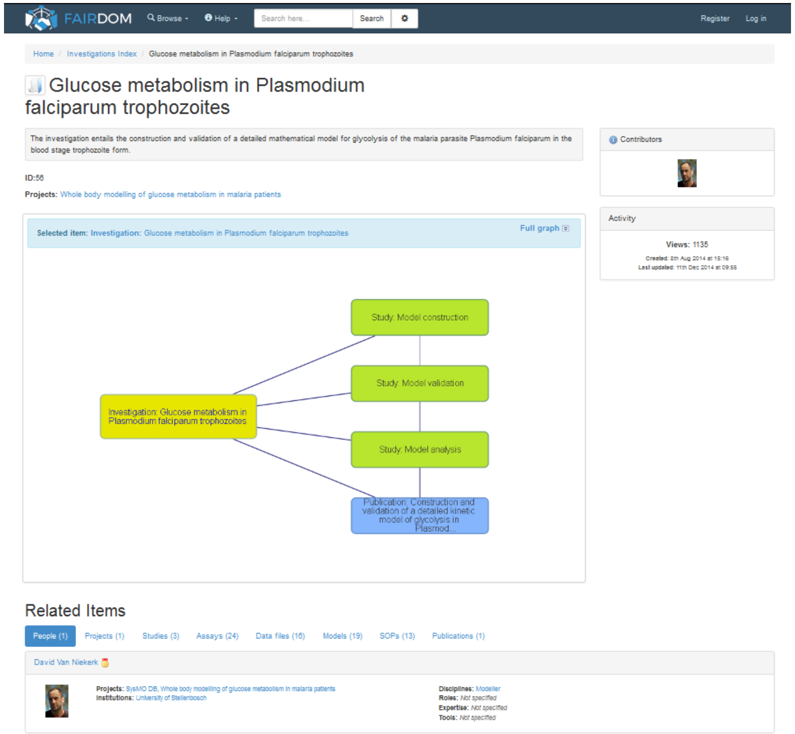
2 Abbreviations

***enzymes*: ALD, fructose-bisp
3-phosphate dehydrogenase (
phosphate dehydrogenase (EC
6-phosphate isomerase (EC
PFK, 6-phosphofructokinase
2.7.2.3); PGM, phosphoglyc**

---

*corresponding author,
[1] Department of Biochemistry, Stellen
jls@sun.ac.za, phone: +27218085844, fa
dam, The Netherlands; [3] MIB, Univers

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



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 modelling of glucose metabolism in malaria patients

Contributors

Activity

Views: 1135

Created: 8th Aug 2014 at 15:16
Last updated: 11th Dec 2014 at 09:55

Selected item: Investigation: Glucose metabolism in Plasmodium falciparum trophozoites

Related Items

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

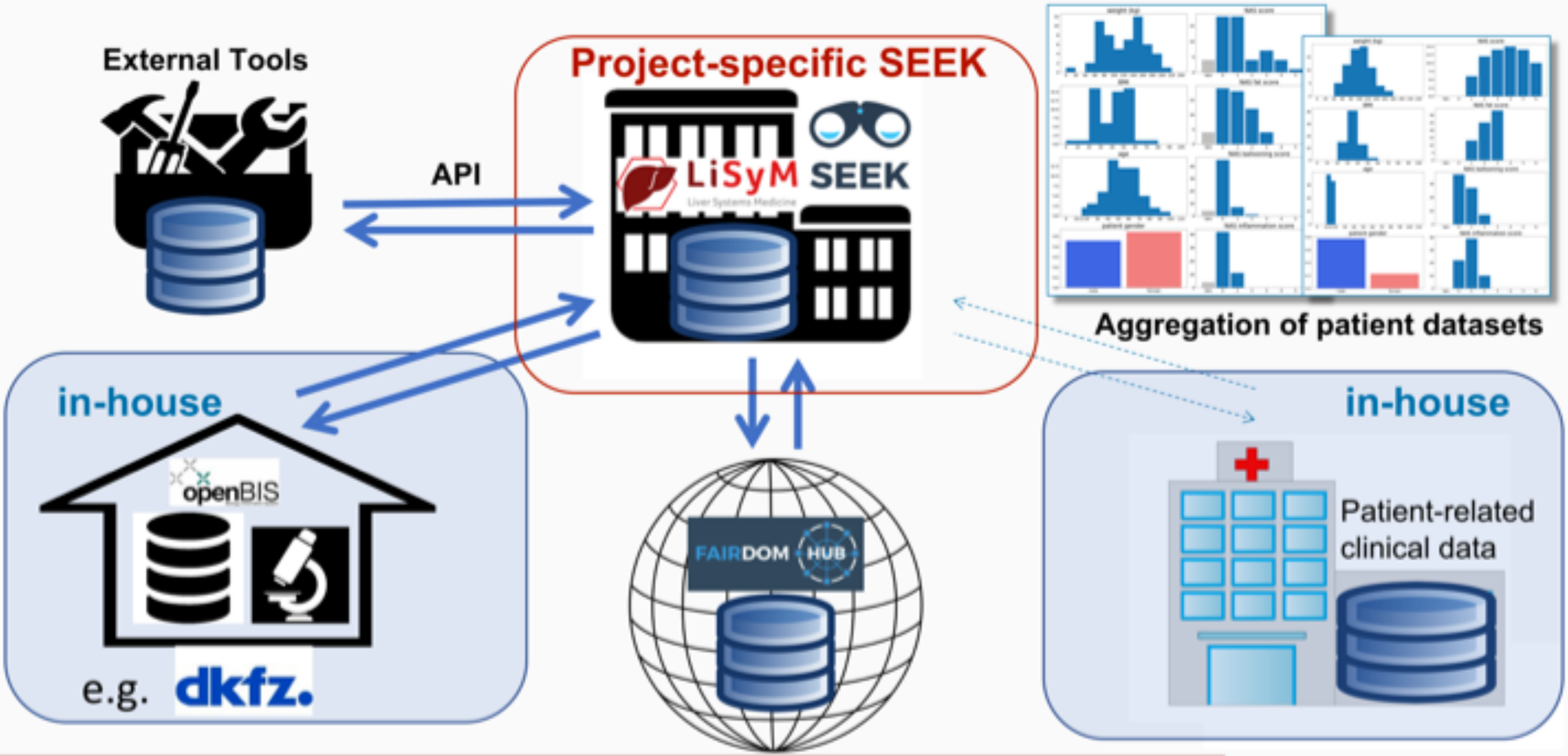
David Van Niekerk

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

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

Penkler et al (2015) FEBSJ 282:1481-1511
[Snoep, 2015]

Project-specific support:
German Liver Systems Medicine Network (LiSyM)



External Tools

API

Project-specific SEEK

Aggregation of patient datasets

in-house

e.g.

in-house

Patient-related clinical data

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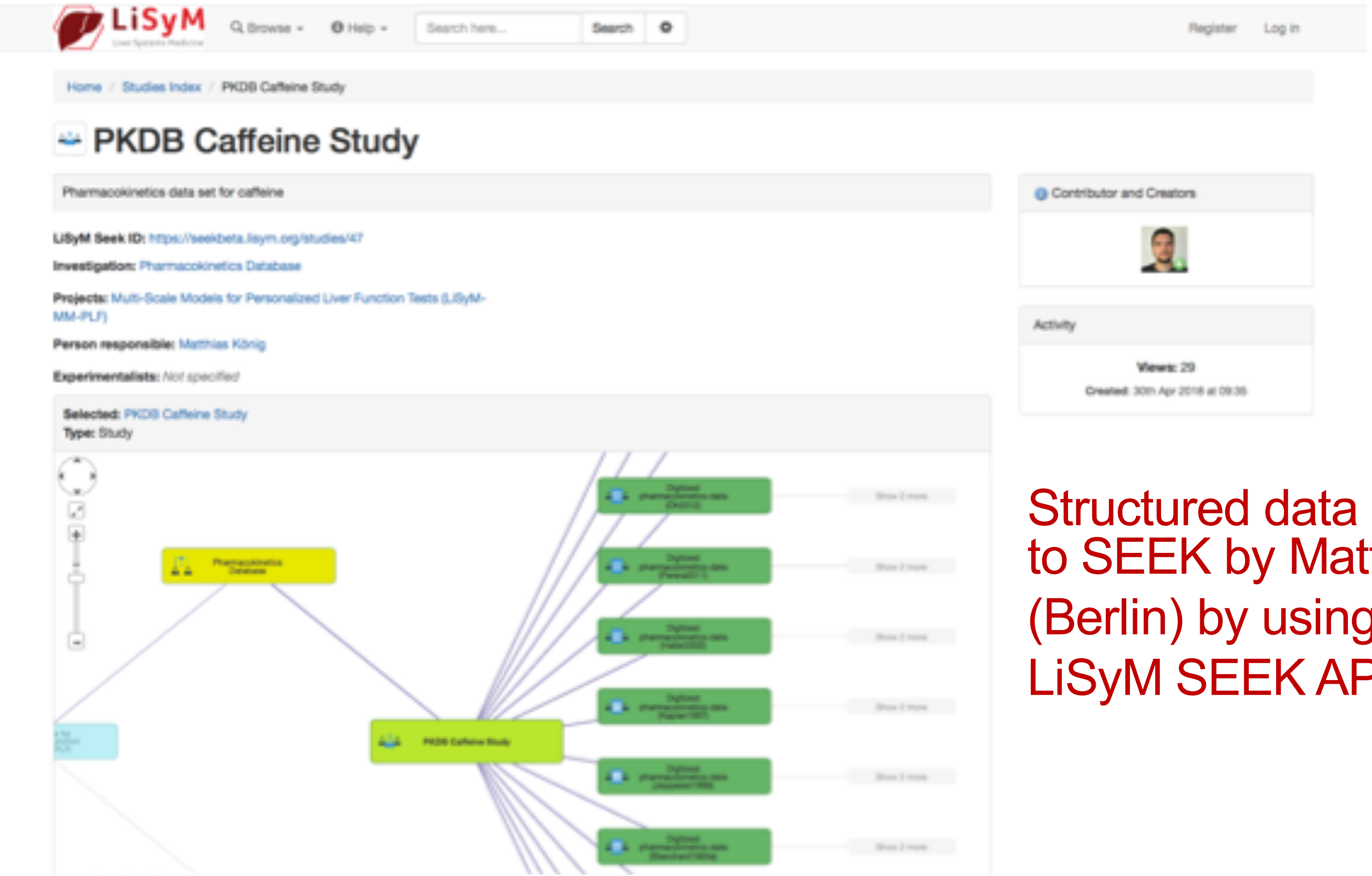
de.NBI

ERASysAPP
ERA-Net for Applied Systems Biology

LiSyM

Federal Ministry of Education and Research

LiSyM SEEK: Programmatic access (API)



PKDB Caffeine Study

Pharmacokinetics data set for caffeine

LiSyM Seek ID: https://seekbeta.lisym.org/studies/47

Investigation: Pharmacokinetics Database

Projects: Multi-Scale Models for Personalized Liver Function Tests (LiSyM-MM-PLF)

Person responsible: Matthias König

Experimentalists: *Not specified*

Selected: PKDB Caffeine Study
Type: Study

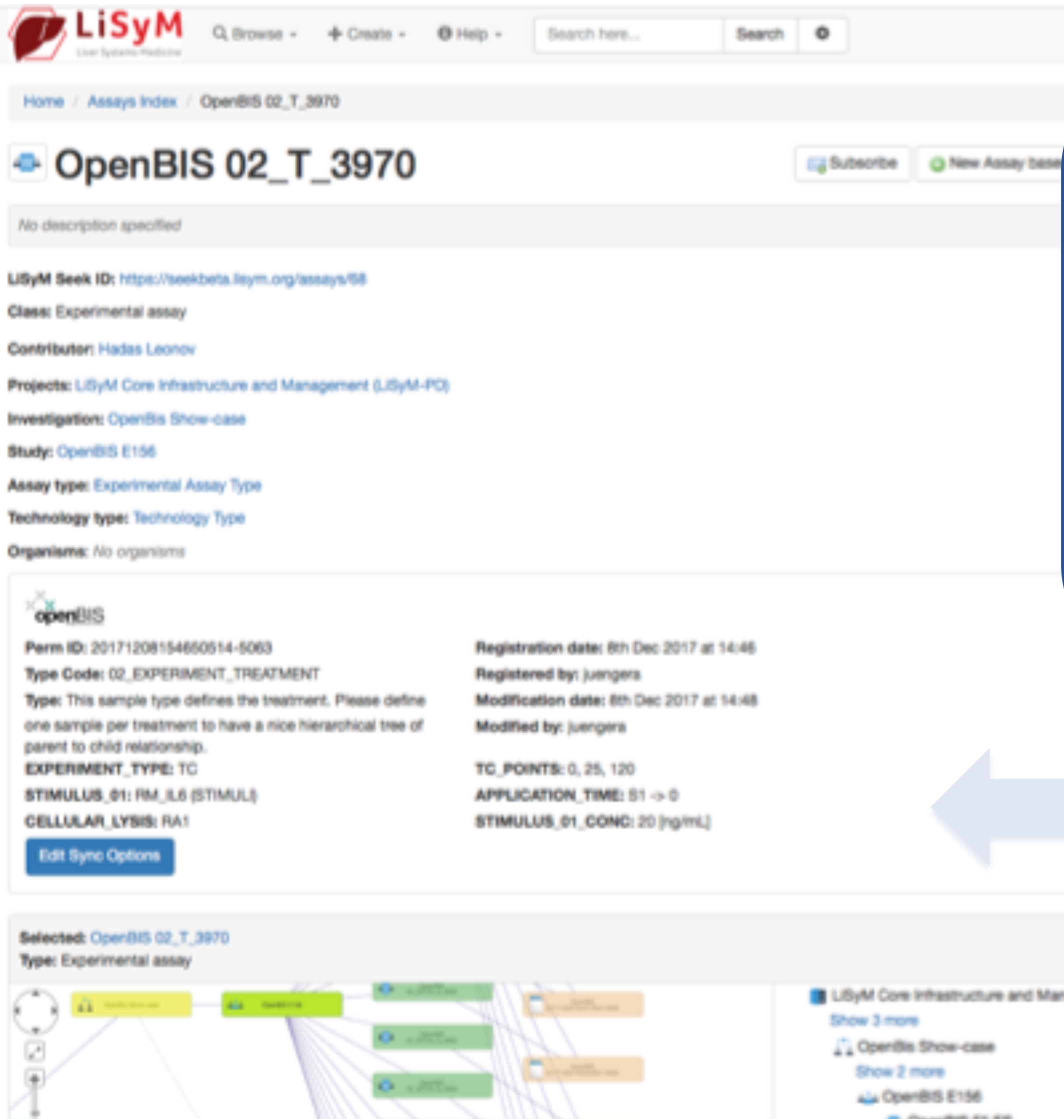
Contributor and Creators

Activity

Views: 29
Created: 30th Apr 2018 at 09:35

Structured data transfered to SEEK by Matthias König (Berlin) by using the LiSyM SEEK API

Integration of data into SEEK from external resources (e.g. openBIS instance at DKFZ for LiSyM)



OpenBIS 02_T_3970

No description specified

LiSyM Seek ID: https://seekbeta.lisym.org/assays/58

Class: Experimental assay

Contributor: Hadas Leonov

Projects: LiSyM Core Infrastructure and Management (LiSyM-PO)

Investigation: OpenBis Show-case

Study: OpenBIS E156

Assay type: Experimental Assay Type

Technology type: Technology Type

Organisms: *No organisms*

openBIS

Perm ID: 20171208154650514-5063

Type Code: 02_EXPERIMENT_TREATMENT

Type: This sample type defines the treatment. Please define one sample per treatment to have a nice hierarchical tree of parent to child relationship.

EXPERIMENT_TYPE: TC

STIMULUS_01: RM_IL6 (STIMULI)

CELLULAR_LYSIS: RA1

Registration date: 8th Dec 2017 at 14:46

Registered by: juengera

Modification date: 8th Dec 2017 at 14:48

Modified by: juengera

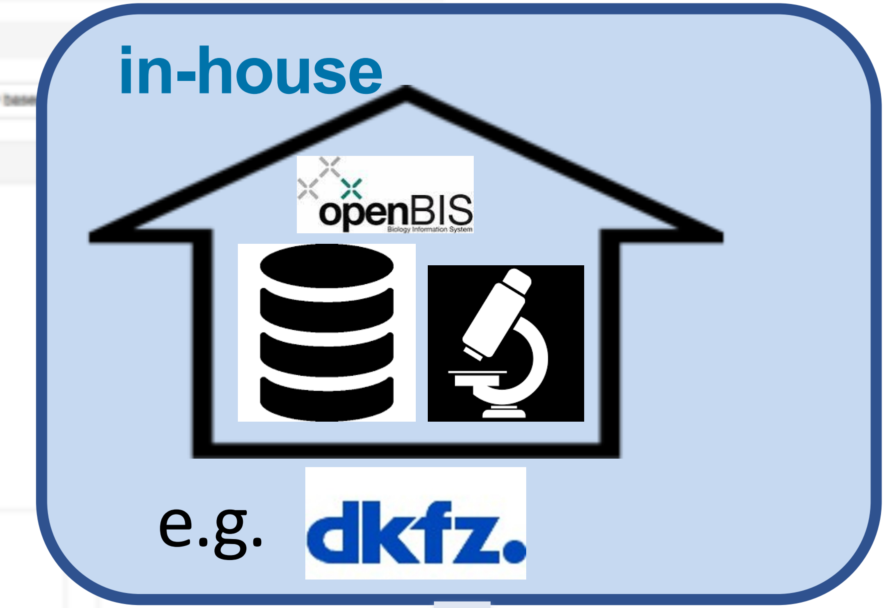
TC_POINTS: 0, 25, 120

APPLICATION_TIME: S1 -> 0

STIMULUS_01_CONC: 20 [ng/mL]

Selected: OpenBIS 02_T_3970

Type: Experimental assay



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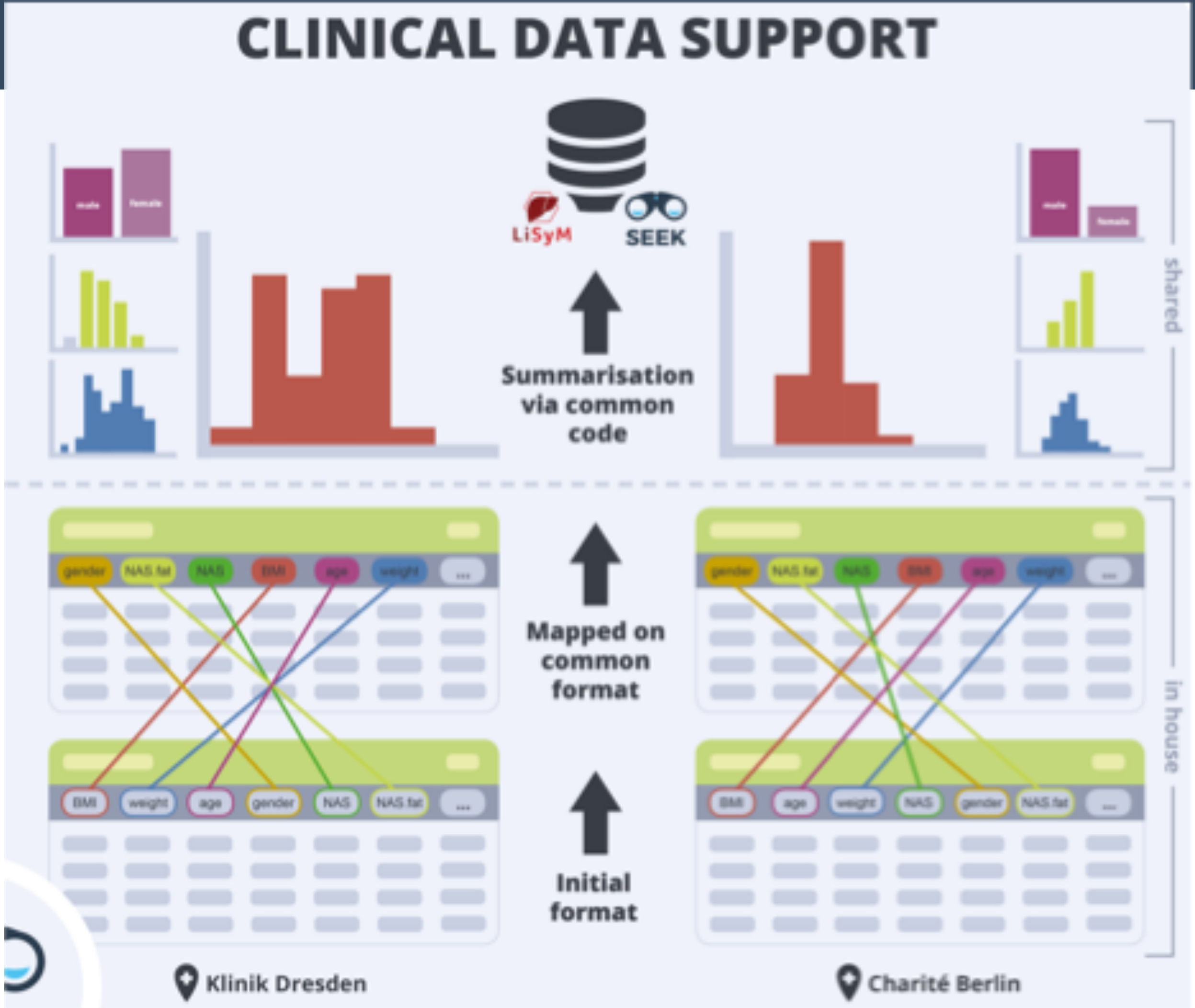
Clinical data sharing concept: e.g. LiSyM clinical data



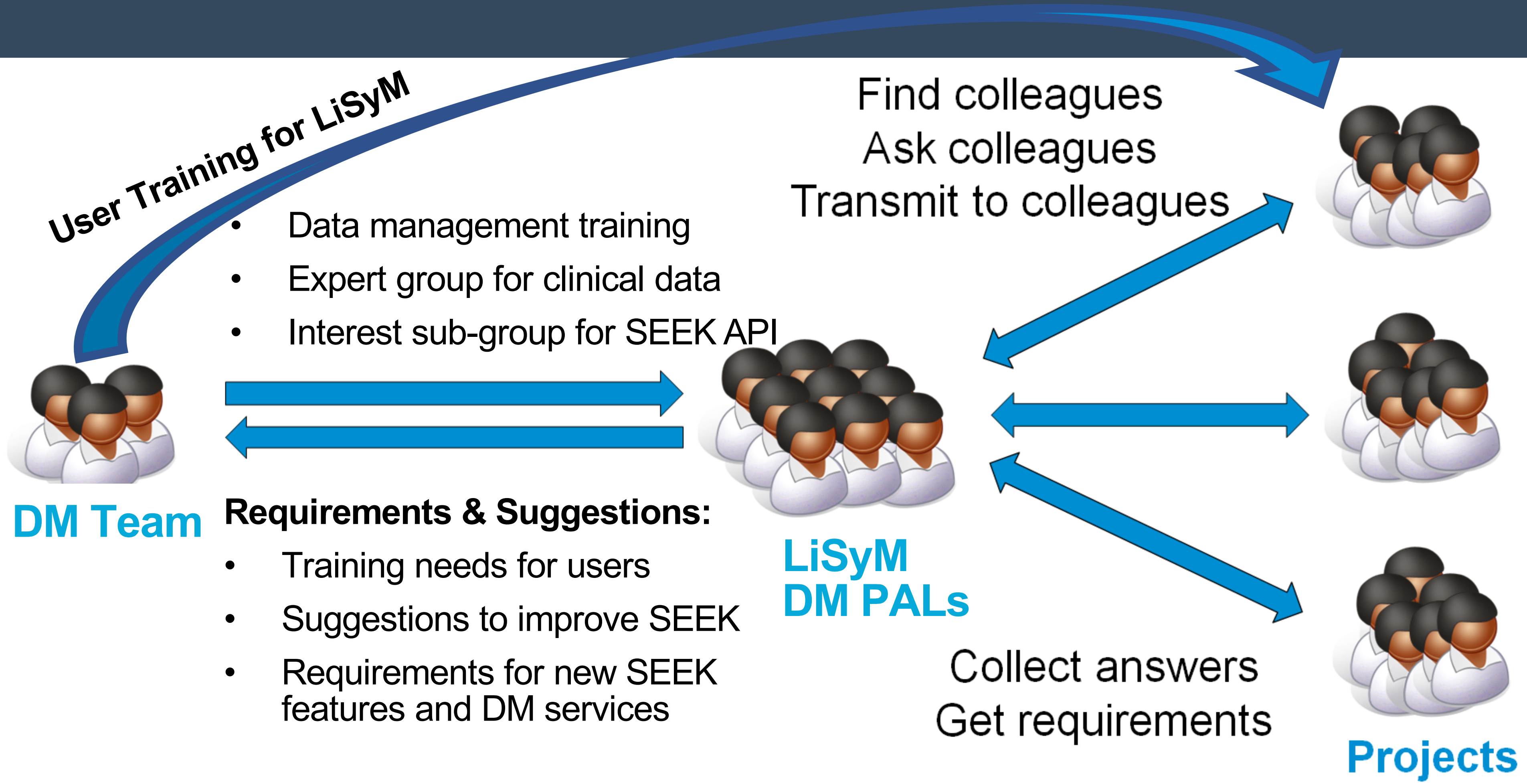
Challenge:

Clinical partners often cannot share person-related data (e.g. for patient samples)

Solution:

- Share table *structure*
- Create & share common code
- Create aggregated summaries (on-site)

Data management PALs - Our advocates in projects



User Training for LiSyM

- Data management training
- Expert group for clinical data
- Interest sub-group for SEEK API

Find colleagues
Ask colleagues
Transmit to colleagues

DM Team

Requirements & Suggestions:

- Training needs for users
- Suggestions to improve SEEK
- Requirements for new SEEK features and DM services

LiSyM
DM PALs

Collect answers
Get requirements

Projects

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ERASysAPP
LiSyM

FAIRDOM TEAM

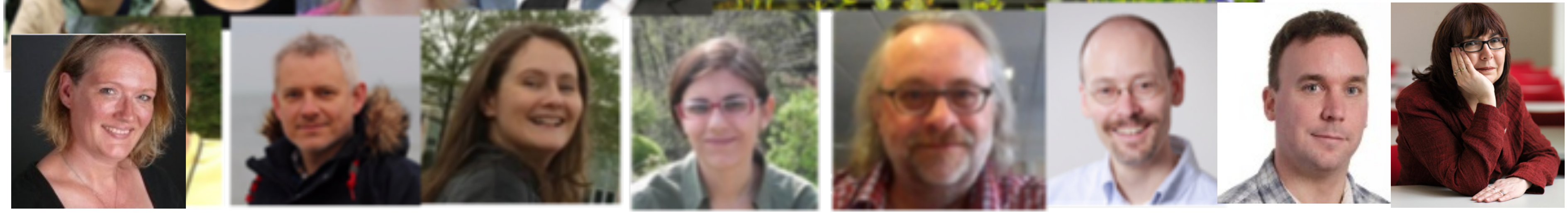
Heidelberg Institute for Theoretical Studies

HITS

MANCHESTER 1824

The University of Manchester

UNIVERSITEIT·STELLENBOSCH·UNIVERSITY
jou kennisvennoot·your knowledge partner



THE FUNDERS

BBSRC

Gabriella Pastori

Adrian Pugh

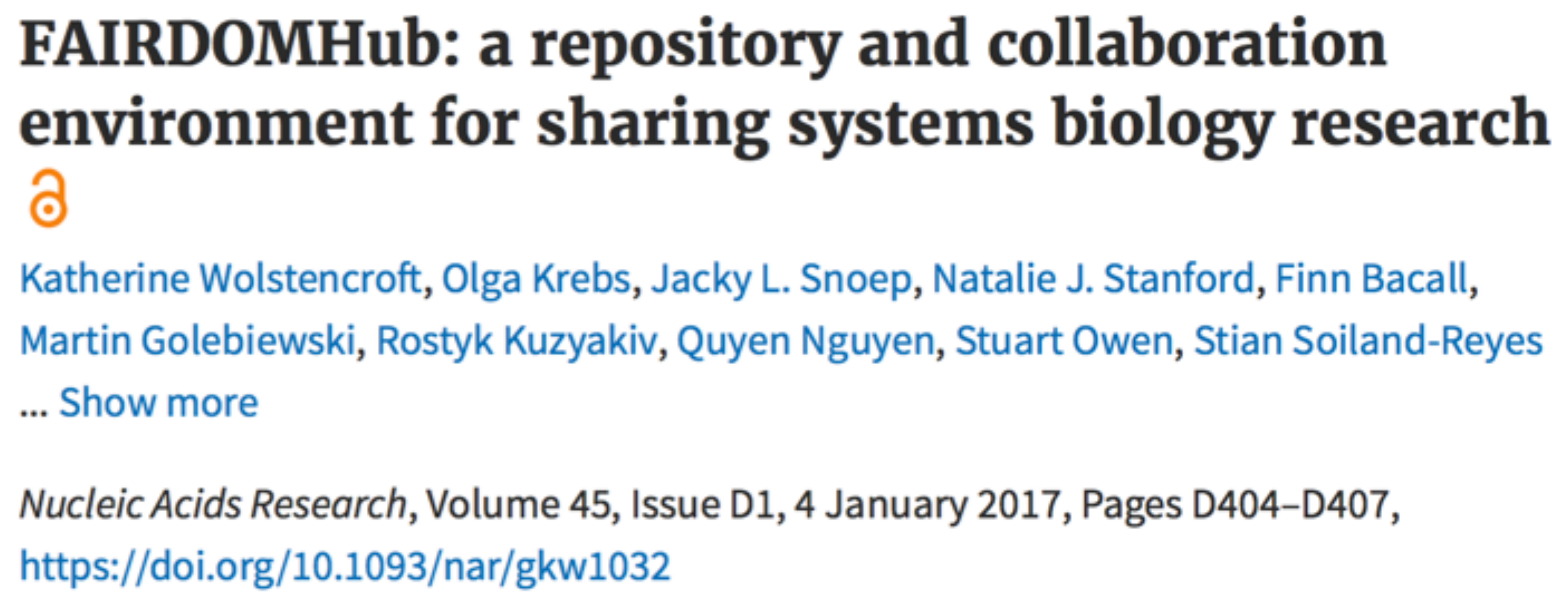
Federal Ministry of Education and Research

PtJ

Christian Ruckert

Petra Schulte

Daniel Vondermuehll



FAIRDOMHub: a repository and collaboration environment for sharing systems biology research

Katherine Wolstencroft, Olga Krebs, Jacky L. Snoep, Natalie J. Stanford, Finn Bacall, Martin Golebiewski, Rostyk Kuzyakiv, Quyen Nguyen, Stuart Owen, Stian Soiland-Reyes ... Show more

Nucleic Acids Research, Volume 45, Issue D1, 4 January 2017, Pages D404–D407,
https://doi.org/10.1093/nar/gkw1032