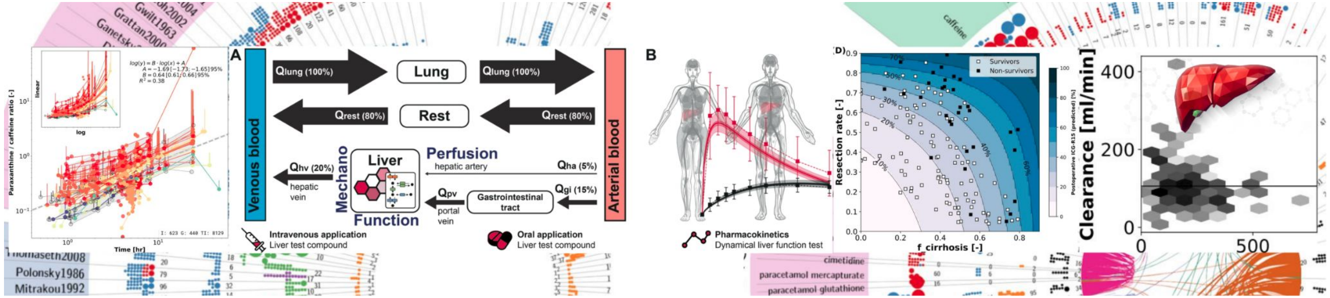


Pharmacokinetics Modeling Course

Reproducible Research & SBML

Dr. Matthias König
Humboldt-University Berlin
Systems Medicine of the Liver
koenigmx@hu-berlin.de
https://livermetabolism.com

🎯 Teaching Goals

By the end of this section, you should be able to:

1. **Understand the role of reproducibility** in computational modeling.
2. **Introduce the Systems Biology Markup Language (SBML)** as a standard for model representation and exchange.
3. **Gain familiarity with tools** for creating,and simulating SBML models (e.g., sbmlutils, cy3sbml).
4. **Discuss FAIR principles** (Findable, Accessible, Interoperable, Reusable) and their application to model data and metadata.
5. **Highlight the importance of open science practices** for transparent and collaborative research.

REPRODUCIBILITY

SCIENTIFIC MEDIA

THIS WEEK

EDITORIALS

Let's think about cognitive bias

The human brain's habit of finding what it wants to find is a key problem for research. Establishing robust methods to avoid such bias will make results more reproducible.

Fewer numbers, better science

Scientific quality is hard to define, and numbers are easy to look at. But bibliometrics are warping science — encouraging quantity over quality. Leaders at two research institutions describe how they do things differently.

Acknowledging and Overcoming Nonrep in Basic and Preclinical Research

dence for nonreproducibility in basic and pre- original study vs 0.71 (95% CI,
iomedical res
from diverse s

COMMENT

nature International weekly journal of science

Home | News & Comment | Research | Careers & Jobs | Current Issue | Archive | Audio &

News & Comment > News > 2016 > May > Article

Reproducibility: Seek out stronger science

Monya Baker

Nature **537**, 703–704

nature

QUALITY TIME

IT MAY NOT BE SEXY, BUT QUALITY ASSURANCE IS BECOMING A CRUCIAL PART OF LAB LIFE.

NATURE | NEWS

Missing mice: gaps in data plague animal rese

Reports of hundreds of biomedical experiments lack essential information.

An open mind on open data

The move to make scientific findings transparent can be a major boon to research, but it can be tricky to embrace the change.

Metrics for ethics

Focus on perceived working conditions could help graduate schools to train responsible researchers.

Hide results to seek the truth

More fields should, like particle physics, adopt blind analysis to thwart bias, urge Robert MacCoun and Saul Perlmutter

Power failure: why small sample size undermines the reliability of neuroscience

Katherine S. Button[1,2], John P. A. Io

Believe it or not: how much rely on published data on po

Repetitive flaws

Strict guidelines to improve the reproducib of experiments are a welcome move.

THIS WEEK

EDITORIALS

Reality check on reproducibility

A survey of Nat results. Resean

ROYAL SOCIETY OPEN SCIENCE

rsos.royalsocietypublishing.org

Research

Low statistical power in biomedical science: a review of three human research domains

NATURE | NEWS

Muddled meanings hamper efforts to fix reproducibility crisis

Researchers tease out different defini

Scientific method: Statistical errors

P values, the 'gold standard' of statistical validity, are not as reliat assume.

Raise standards for preclinical cancer research

THE LANCET

"85% of health research is wasted."

Confidence in preclinical research

For decades, model organisms have provided an important reductionist approach for understanding

making strides in their efforts to understand an for the complexity of the microbiome in rodent

DUE DILIGENCE, OVERDUE

Perrin S (2014) Nature 407:423

Results of rigorous animal tests by the Amyotrophic Lateral Sclerosis Therapy Development Institute (ALS are less promising than those published. All these compounds have disappointed in human testing.

PUBLIC MEDIA

The Breakdown in Biomedical Research

Contaminated samples, faulty studies and have created a crisis in laboratories and in quest for new treatments and cures

Wall Street Journal 7.4.2017

The Economist

Washington's lawyer surplus
How to do a nuclear deal with Iran
Investment tips from Nobel economist
Junk bonds are back
The meaning of Sachin Tendulkar

HOW SCIENCE GOES WRONG

99
Einsteinium

THE NEW YORKER

SUBSCRIBE | IN THE MAGAZINE | BLOGS | AUDIO & VIDEO | LISTINGS

POLITICS | PROFILES | THE TALK OF THE TOWN | COMMENT | TABLE OF CONTENTS | THE FINANCIAL PAGE

ANNALS OF SCIENCE

THE TRUTH WEARS OFF

Is there something wrong with the scientific method?

BY JONAH LEHRER

DECEMBER 13, 2010

FEATURES

How many scientific papers just aren't true?

Enough that basing government policy on 'peer-reviewed studies' isn't all it's cracked up to be

Donna Laframboise

The Economist

Why bad science persists

Incentive malus

Poor scientific methods may be hereditary

Sep 24th 2016 | From the print edition

the Atlantic

November 2010

Lies, Damned Lies, and Medical Science

MUCH OF WHAT MEDICAL RESEARCHERS CONCLUDE IN THEIR STUDIES IS MISLEADING,
FLAT-OUT WRONG. SO WHY ARE DOCTORS—TO A STRIKING EXTENT—STILL DRAWING U
MISINFORMATION IN THEIR EVERYDAY PRACTICE? DR. JOHN IOANNIDIS HAS SPENT HIS
CHALLENGING HIS PEERS BY EXPOSING THEIR BAD SCIENCE.

By David H. Freedman

The New York Times

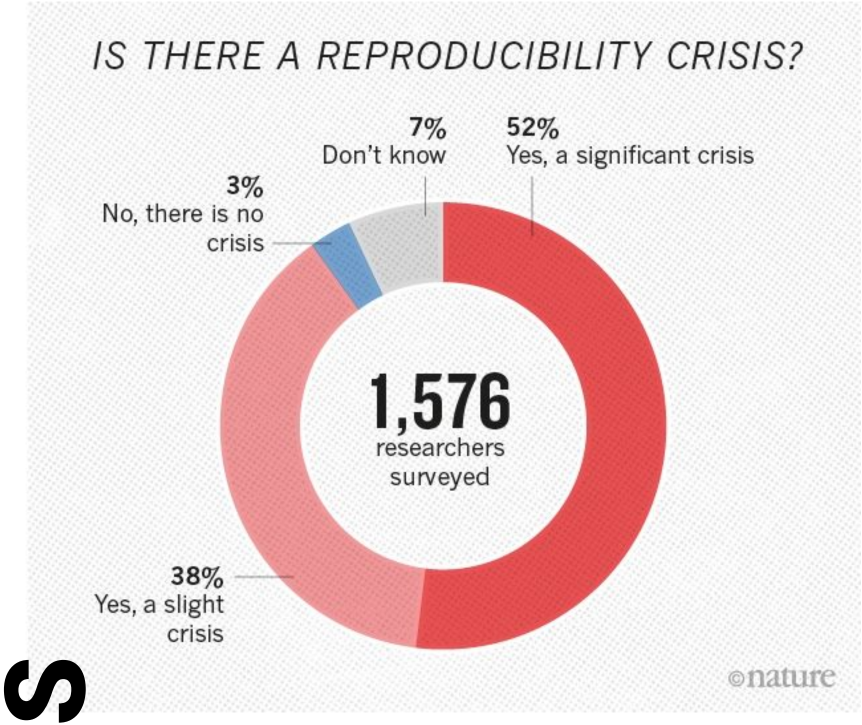
SCIENCE

Science, Now Under Scrutiny Itself

Editorial: "Is science in big trouble?"

The 5th World Conference on Research Integrity will explore the challenges of promoting transparency and accountability in research — and develop an agenda for action

SCIENTISTS



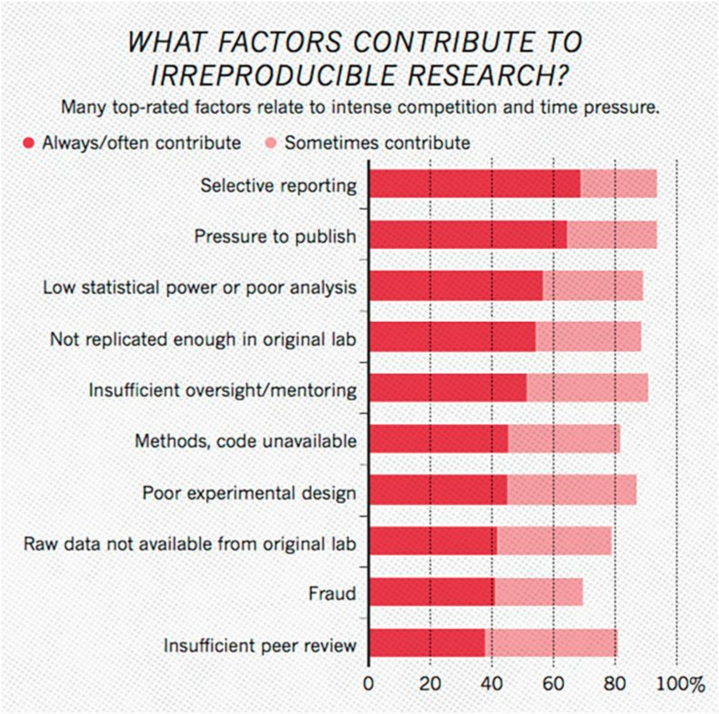
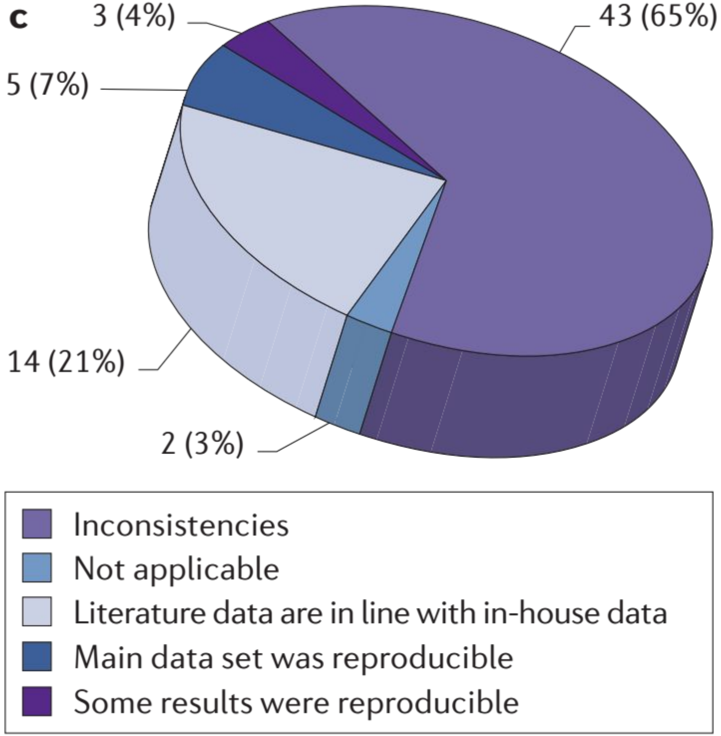


FIGURE 5: Plot Representing What Researchers Believe are the Primary Causes of Reproducibility Failure in the Sciences.

Is there a reproducibility crisis
Baker, Nature May 2016, Vol 533, 453

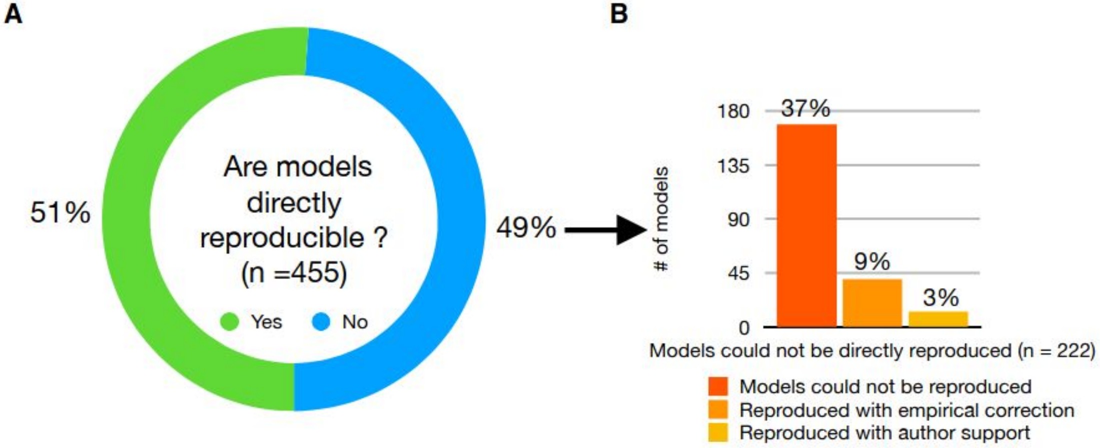
Industry Efforts

- **Amgen (6/53) & Bayer (14/67)**
- **Bayer halts nearly two-thirds of its target-validation projects** because in-house experimental findings fail to match up with published literature claims
- internal experiments matched up with the published findings in only 14 projects, but were **highly inconsistent in 43/67**



Believe it or not: how much can we rely on published data on potential drug targets? - Nature Reviews Drug Discovery 10, 643-644 (2011)

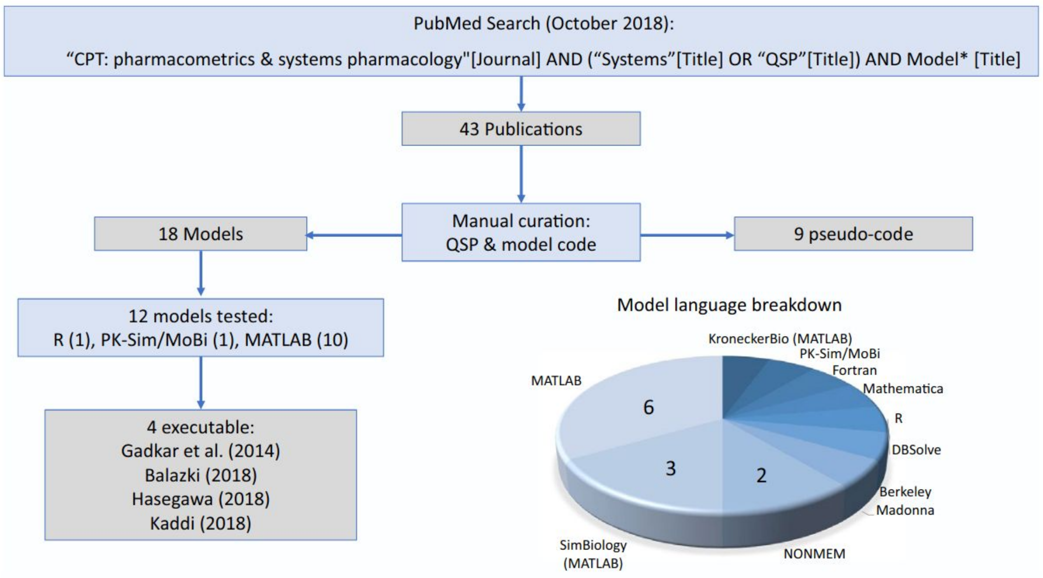
Reproducibility of Computational Models



- Most models not accessible
- Many accessible models not reproducible

Tiwari K, Kananathan S, Roberts MG, Meyer JP, Sharif Shohan MU, Xavier A, Maire M, Zyoud A, Men J, Ng S, Nguyen TVN, Glont M, Hermjakob H, Malik-Sheriff RS. Reproducibility in systems biology modelling. Mol Syst Biol. 2021 Feb;17(2):e9982. doi: 10.15252/msb.20209982. PMID: 33620773; PMCID: PMC7901289.

Reproducibility of Computational Models



PubMed Search (October 2018):

“CPT: pharmacometrics & systems pharmacology"[Journal] AND (“Systems”[Title] OR “QSP”[Title]) AND Model* [Title]

43 Publications

Manual curation:
QSP & model code

18 Models

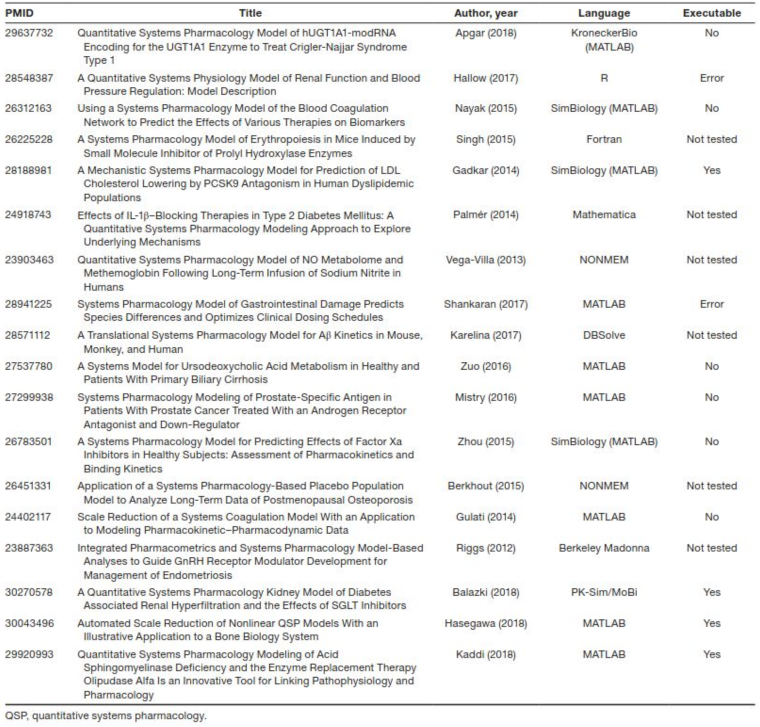
9 pseudo-code

12 models tested:
R (1), PK-Sim/MoBi (1), MATLAB (10)

4 executable:
Gadkar et al. (2014)
Balazki (2018)
Hasegawa (2018)
Kaddi (2018)

Figure 1 Workflow and results summary. QSP, quantitative systems pharmacology.

Table 1 Summary of 18 QSP models

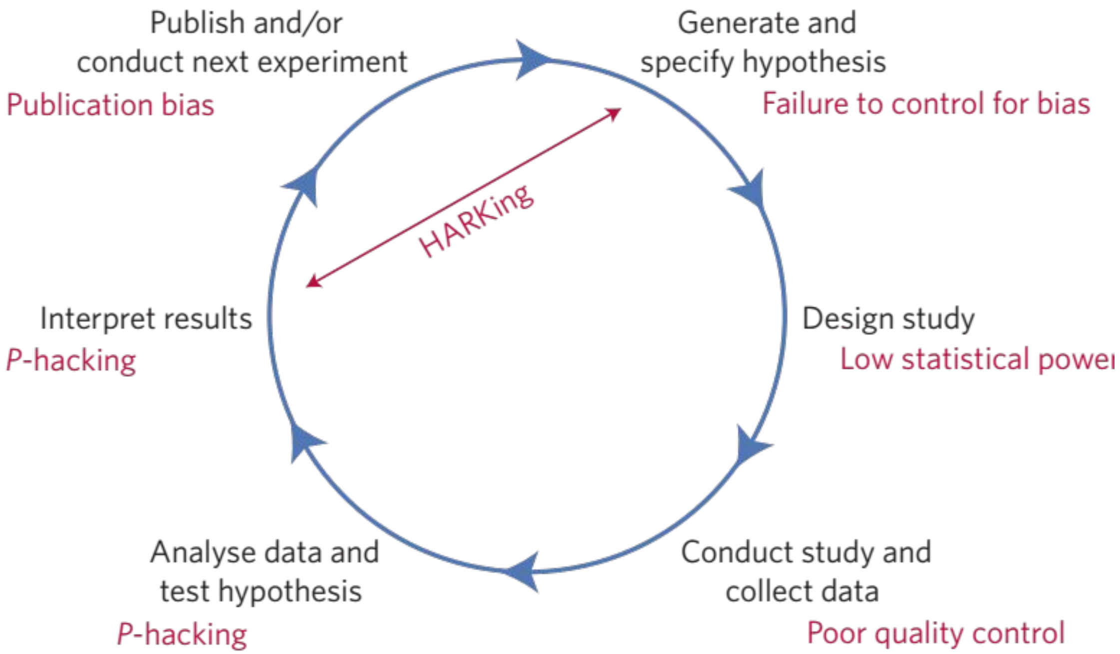


PMID	Title	Author, year	Language	Executable
29637732	Quantitative Systems Pharmacology Model of hUGT1A1-modRNA Encoding for the UGT1A1 Enzyme to Treat Crigler-Najjar Syndrome Type 1	Apgar (2018)	KroneckerBio (MATLAB)	No
28548387	A Quantitative Systems Physiology Model of Renal Function and Blood Pressure Regulation: Model Description	Hallow (2017)	R	Error
26312163	Using a Systems Pharmacology Model of the Blood Coagulation Network to Predict the Effects of Various Therapies on Biomarkers	Nayak (2015)	SimBiology (MATLAB)	No
26225228	A Systems Pharmacology Model of Erythropoiesis in Mice Induced by Small Molecule Inhibitor of Prolyl Hydroxylase Enzymes	Singh (2015)	Fortran	Not tested
28188981	A Mechanistic Systems Pharmacology Model for Prediction of LDL Cholesterol Lowering by PCSK9 Antagonism in Human Dyslipidemic Populations	Gadkar (2014)	SimBiology (MATLAB)	Yes
24918743	Effects of IL-1β–Blocking Therapies in Type 2 Diabetes Mellitus: A Quantitative Systems Pharmacology Modeling Approach to Explore Underlying Mechanisms	Palmér (2014)	Mathematica	Not tested
23903463	Quantitative Systems Pharmacology Model of NO Metabolome and Methemoglobin Following Long-Term Infusion of Sodium Nitrite in Humans	Vega-Villa (2013)	NONMEM	Not tested
28941225	Systems Pharmacology Model of Gastrointestinal Damage Predicts Species Differences and Optimizes Clinical Dosing Schedules	Shankaran (2017)	MATLAB	Error
28571112	A Translational Systems Pharmacology Model for Aβ Kinetics in Mouse, Monkey, and Human	Karelina (2017)	DBSolve	Not tested
27537780	A Systems Model for Ursodeoxycholic Acid Metabolism in Healthy and Patients With Primary Biliary Cirrhosis	Zuo (2016)	MATLAB	No
27299938	Systems Pharmacology Modeling of Prostate-Specific Antigen in Patients With Prostate Cancer Treated With an Androgen Receptor Antagonist and Down-Regulator	Mistry (2016)	MATLAB	No
26783501	A Systems Pharmacology Model for Predicting Effects of Factor Xa Inhibitors in Healthy Subjects: Assessment of Pharmacokinetics and Binding Kinetics	Zhou (2015)	SimBiology (MATLAB)	No
26451331	Application of a Systems Pharmacology-Based Placebo Population Model to Analyze Long-Term Data of Postmenopausal Osteoporosis	Berkhout (2015)	NONMEM	Not tested
24402117	Scale Reduction of a Systems Coagulation Model With an Application to Modeling Pharmacokinetic–Pharmacodynamic Data	Gulati (2014)	MATLAB	No
23887363	Integrated Pharmacometrics and Systems Pharmacology Model-Based Analyses to Guide GnRH Receptor Modulator Development for Management of Endometriosis	Riggs (2012)	Berkeley Madonna	Not tested
30270578	A Quantitative Systems Pharmacology Kidney Model of Diabetes Associated Renal Hyperfiltration and the Effects of SGLT Inhibitors	Balazki (2018)	PK-Sim/MoBi	Yes
30043496	Automated Scale Reduction of Nonlinear QSP Models With an Illustrative Application to a Bone Biology System	Hasegawa (2018)	MATLAB	Yes
29920993	Quantitative Systems Pharmacology Modeling of Acid Sphingomyelinase Deficiency and the Enzyme Replacement Therapy Olipudase Alfa Is an Innovative Tool for Linking Pathophysiology and Pharmacology	Kaddi (2018)	MATLAB	Yes

QSP, quantitative systems pharmacology.

Kirouac DC, Cicali B, Schmidt S. Reproducibility of Quantitative Systems Pharmacology Models: Current Challenges and Future Opportunities. CPT Pharmacometrics Syst Pharmacol. 2019 Apr;8(4):205-210. doi: 10.1002/psp4.12390. Epub 2019 Mar 3. PMID: 30697975; PMCID: PMC6482280.

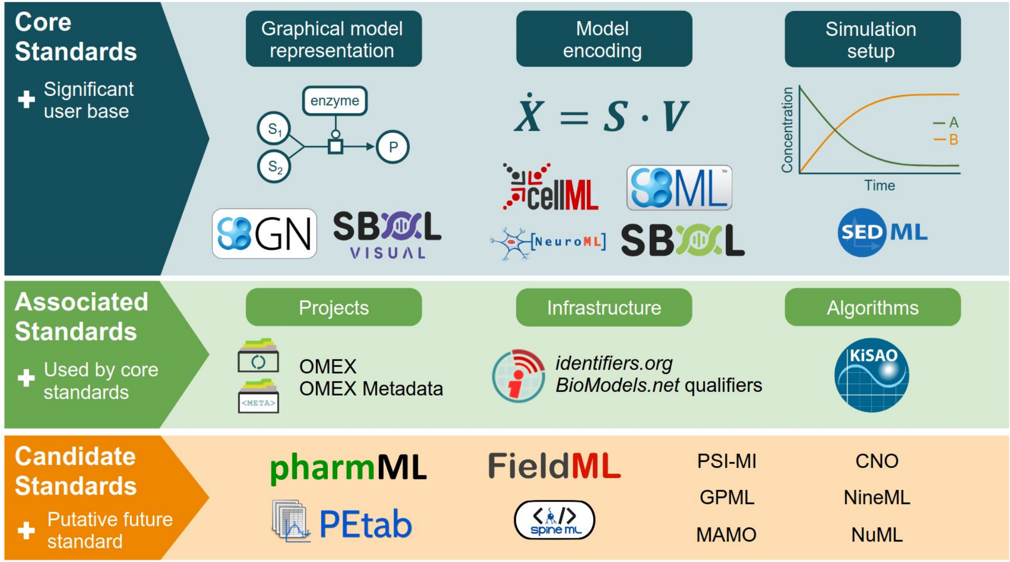
Threats to Scientific Method



- Poor study design
- Low statistical power
- Analytical flexibility
- P-hacking
- Hypothesizing after the results are known (HARKing)
- Publication bias
- Lack of data sharing

Munafò MR, Nosek BA, Bishop DVM, Button KS, Chambers CD, du Sert NP, Simonsohn U, Wagenmakers EJ, Ware JJ, Ioannidis
2017 Jan 10;1(1):0021. doi: 10.1038/s41562-016-0021. PMID: 33954258; PMCID: PMC7610724.

Development of Standards



Core Standards

+ Significant user base

Graphical model representation

Model encoding

$\dot{X} = S \cdot V$

Simulation setup

Associated Standards

+ Used by core standards

Projects

OMEX
OMEX Metadata

Infrastructure

identifiers.org
BioModels.net qualifiers

Algorithms

Candidate Standards

+ Putative future standard

pharmML
PEtab
FieldML
PSI-MI
GPML
MAMO
CNO
NineML
NuML

- Models (SBML)
- Simulationen (SED-ML)
- Visualisation (SGBN)
- Parameter Optimization (PETab)
- Metadata (OMEX)
- COMBINE archive

Specifications of Standards in Systems and Synthetic Biology: Status and Developments in 2022 and the COMBINE meeting 2022. **M. König** et al. J Integr Bioinform. 2023 Mar 29;20(1).

SBML Level 3: an extensible format for the exchange and reuse of biological models. SM Keating, D Waltemath, **M König**, ..., M Hucka, and SBML Community members. Mol Syst Biol. 2020;16(8):e9110. doi:10.15252/msb.20199110

The Systems Biology Markup Language (SBML): Language Specification for Level 3 Version 2 Core. M. Hucka, F. Bergmann, C. Chaouiya, A. Dräger, S. Hoops, S. Keating, **M. König**, N Le Novere, C. Myers, B. Olivier, S. Sahle, J. Schaff, R. Sheriff, L. Smith, D. Waltemath, D. Wilkinson, F. Zhang. J Integr Bioinform. 2019 Jun 20;16(2); 10.1515/jib-2019-0021

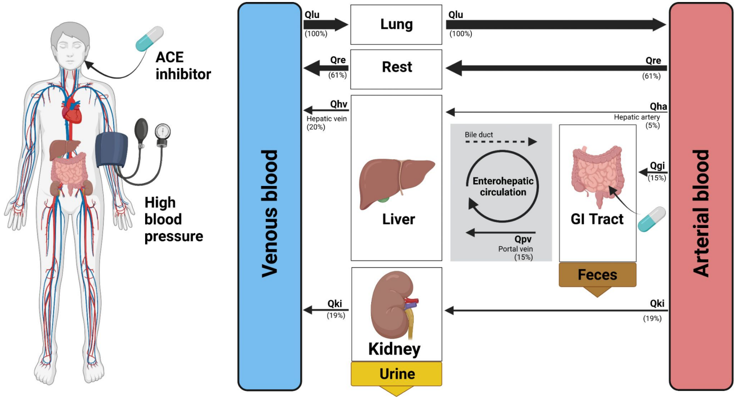
The Distributions Package for SBML Level 3. L Smith, S Moodie, F Bergmann, C Gillespie, S Keating, **M. König**, C Myers, M Swat, D Wilkinson, M Hucka. J Integr Bioinform. 2020 Aug 4; doi: 10.1515/jib-2020-0018

Open modeling and exchange (OMEX) metadata specification version 1.0. Neal ML, Gennari JH, Waltemath D, Nickerson DP, **König M.** J Integr Bioinform. 2020 Jun 25;17(2-3):20200020. doi:10.1515/jib-2020-0020.

Harmonizing semantic annotations for computational models in biology. Neal, M.; **König,** M.; Nickerson, D., ...mWaltemath, D. Brief Bioinform. 2019 Mar 22;20(2):540-550. doi:10.1093/bib/bby087.

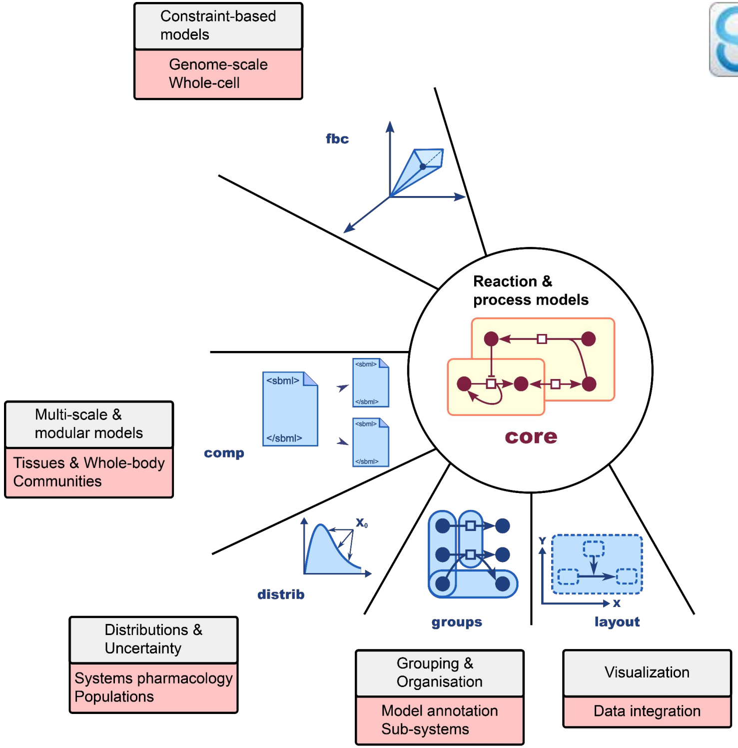
Systems Biology Markup Language (SBML)

- SBML is a software data format for describing models in biology (https://sbml.org)
- It's a little like HTML but for model instead of web pages
- independent of any particular tool
- free and open
- De facto standard



SBML

- **Process-based ODE models**
- Reproducible & exchangeable model encoding (**SBML**)
- Annotations to modelling, biological and medical ontologies (**SBML core**)
- Hierarchical models/multi-scale models
- (**SBML comp**)
- Unit validation, unit checking, unit conversion
- Distributions in models & uncertainty in data and parameters (**SBML distrib**)
- Mass- & charge balance (**SBML fbc**)
- Use wide range of tools (visualization, parameter fitting, simulation, ...)
- http://sbml.org



Constraint-based models

Genome-scale
Whole-cell

Multi-scale & modular models

Tissues & Whole-body
Communities

Distributions & Uncertainty

Systems pharmacology
Populations

Grouping & Organisation

Model annotation
Sub-systems

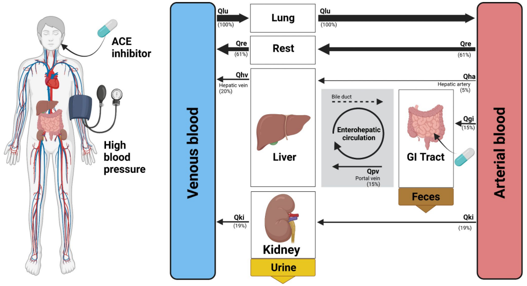
Visualization

Data integration

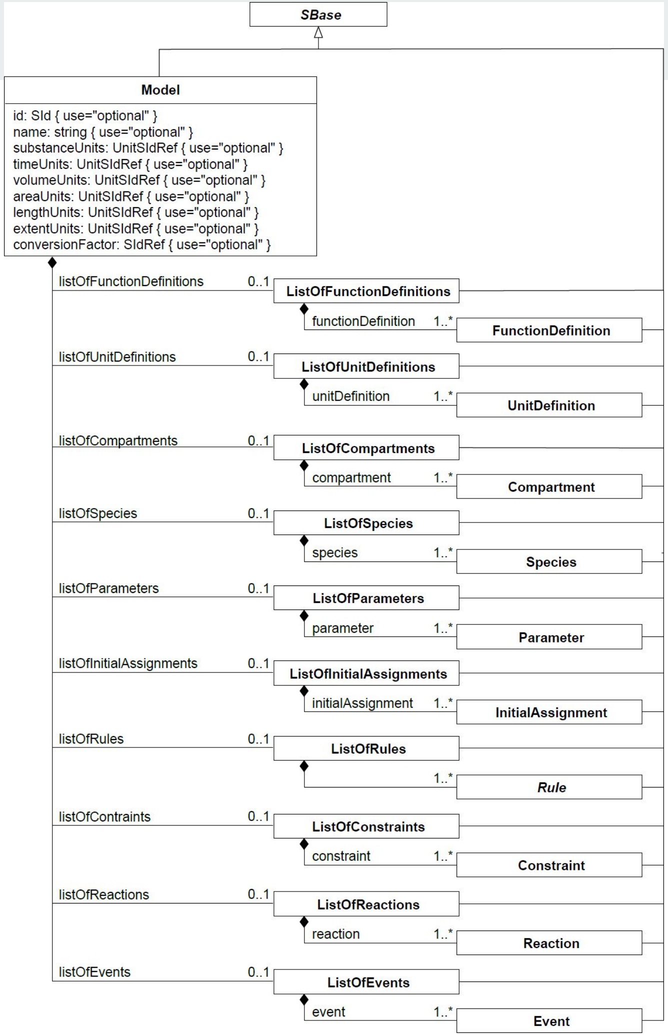
Reaction & process models

Keating SM, Waltemath D, König M, ... , Hucka M; SBML Level 3 Community members. SBML Level 3: an extensible format for the exchange and reuse of biological models. Mol Syst Biol. 2020 Aug;16(8):e9110. doi: 10.15252/msb.20199110.

SBML core



- Compartments
  - containers/volumes (e.g. liver volume)
- Species
  - molecules in compartments (e.g. `glucose` in plasma)
- Parameters
  - parameters with values (e.g. `cardiac output`)
- AssignmentRules
  - mathematical relationships between other parameters, species, compartments (e.g. `BMI = bodyweight/height`^{2})
- Reactions
  - processes converting species in other species (e.g. enzymatic conversion; e.g. transport via blood flow)



sbmlutils: Python Utilities for Working with SBML

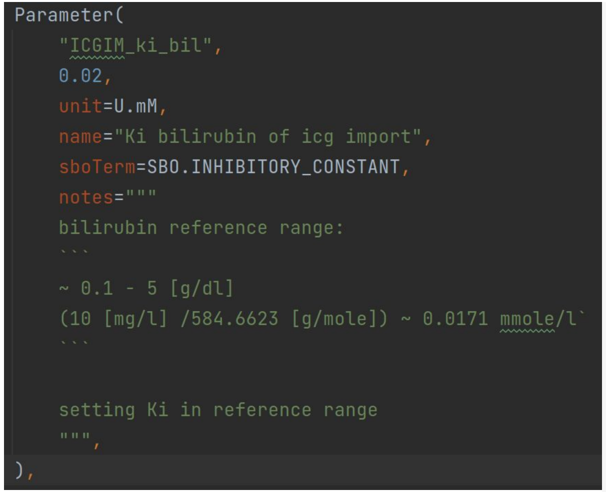
https://github.com/matthiaskoenig/sbmlutils

Packages

- core, fbc, comp, distrib, layout

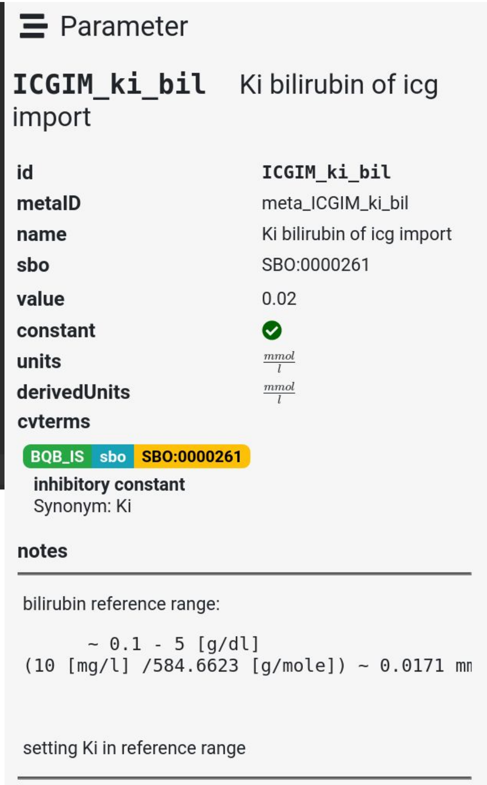
Features

- model creation, manipulation & merging
- unit support
- model annotation
- interpolations
- file converters (XPP)
- markdown annotations
- OMEX support



~~~
Parameter(
    "ICGIM_ki_bil",
    0.02,
    unit=U.mM,
    name="Ki bilirubin of icg import",
    sboTerm=SBO.INHIBITORY_CONSTANT,
    notes="""
    bilirubin reference range:
    ```
    ~ 0.1 - 5 [g/dl]
    (10 [mg/l] /584.6623 [g/mole]) ~ 0.0171 mmole/l`
    ```


    setting Ki in reference range
    """,
),
~~~



`ICGIM_ki_bil` Ki bilirubin of icg import

id	**`ICGIM_ki_bil`**
metaID	meta_ICGIM_ki_bil
name	Ki bilirubin of icg import
sbo	SBO:0000261
value	0.02
constant	✓
units	$\frac{mmol}{l}$
derivedUnits	$\frac{mmol}{l}$
cvterms	

BQB_IS sbo SBO:0000261

inhibitory constant
Synonym: Ki

notes

bilirubin reference range:

```
    ~ 0.1 - 5 [g/dl]
(10 [mg/l] /584.6623 [g/mole]) ~ 0.0171 mm
```

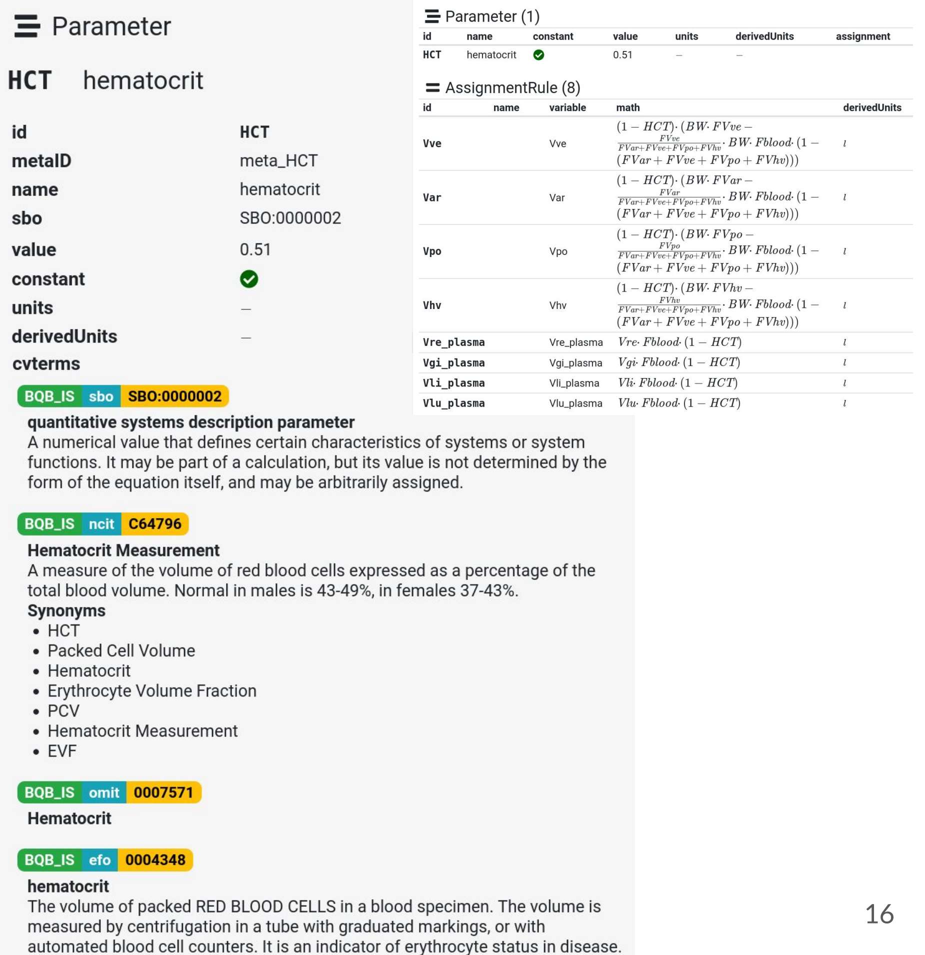
setting Ki in reference range

SBML4Humans: Human Readable SBML Report

https://sbml4humans.de

- **interactive SBML report** with navigation between SBML objects
- **web application** (no setup)
- **search** and filter functionality
- **resolve/render metadata**
- **hierarchical models** (SBML comp)
- **distributions and uncertainties** (SBML distrib)
- **flux balance** (SBML fbc)
- **COMBINE archives** (multiple models)
- **URL endpoint** for integration in tools/ workflows/ webpages/ presentations

[`https://sbml4humans.de/model_url?url=https://www.ebi.ac.uk/biomodels/model/download/BIOMD0000000001.2?filename=BIOMD0000000001_url.xml`](https://sbml4humans.de/model_url?url=https://www.ebi.ac.uk/biomodels/model/download/BIOMD0000000001.2?filename=BIOMD0000000001_url.xml)



Parameter

HCT hematocrit

id	HCT
metaID	meta_HCT
name	hematocrit
sbo	SBO:0000002
value	0.51
constant	✓
units	–
derivedUnits	–
cvterms	

BQB_IS sbo SBO:0000002

quantitative systems description parameter
A numerical value that defines certain characteristics of systems or system functions. It may be part of a calculation, but its value is not determined by the form of the equation itself, and may be arbitrarily assigned.

BQB_IS ncit C64796

Hematocrit Measurement
A measure of the volume of red blood cells expressed as a percentage of the total blood volume. Normal in males is 43-49%, in females 37-43%.
Synonyms

- HCT
- Packed Cell Volume
- Hematocrit
- Erythrocyte Volume Fraction
- PCV
- Hematocrit Measurement
- EVF

BQB_IS omit 0007571

Hematocrit

BQB_IS efo 0004348

hematocrit
The volume of packed RED BLOOD CELLS in a blood specimen. The volume is measured by centrifugation in a tube with graduated markings, or with automated blood cell counters. It is an indicator of erythrocyte status in disease.

Parameter (1)

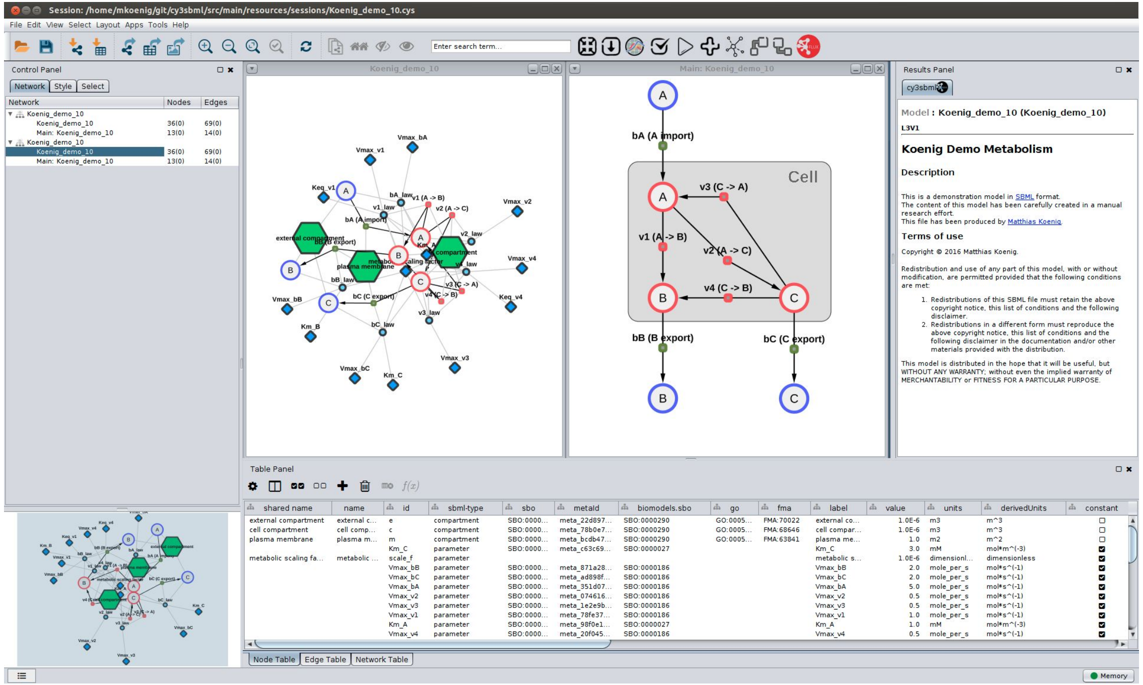
id	name	constant	value	units	derivedUnits	assignment
HCT	hematocrit	✓	0.51	–	–	

AssignmentRule (8)

id	name	variable	math	derivedUnits
Vve		Vve	$(1-HCT)\cdot(BW\cdot FVve-\frac{FVve}{FVar+FVve+FVpo+FVhv}\cdot BW\cdot Fblood\cdot(1-(FVar+FVve+FVpo+FVhv)))$	l
Var		Var	$(1-HCT)\cdot(BW\cdot FVar-\frac{FVar}{FVar+FVve+FVpo+FVhv}\cdot BW\cdot Fblood\cdot(1-(FVar+FVve+FVpo+FVhv)))$	l
Vpo		Vpo	$(1-HCT)\cdot(BW\cdot FVpo-\frac{FVpo}{FVar+FVve+FVpo+FVhv}\cdot BW\cdot Fblood\cdot(1-(FVar+FVve+FVpo+FVhv)))$	l
Vhv		Vhv	$(1-HCT)\cdot(BW\cdot FVhv-\frac{FVhv}{FVar+FVve+FVpo+FVhv}\cdot BW\cdot Fblood\cdot(1-(FVar+FVve+FVpo+FVhv)))$	l
Vre_plasma		Vre_plasma	$Vre\cdot Fblood\cdot(1-HCT)$	l
Vgi_plasma		Vgi_plasma	$Vgi\cdot Fblood\cdot(1-HCT)$	l
Vli_plasma		Vli_plasma	$Vli\cdot Fblood\cdot(1-HCT)$	l
Vlu_plasma		Vlu_plasma	$Vlu\cdot Fblood\cdot(1-HCT)$	l

CySBML: Cytoscape app for visualizing SBML

- **kinetic & reaction-species view**
- **subgraphs & filtering**
- **annotation support**
- **works for large scale networks** (genome-scale)
- **sbmlutils integration** (py4cytoscape)



Network	Nodes	Edges
Koenig_demo_10		
Koenig_demo_10	36(0)	69(0)
Main: Koenig_demo_10	13(0)	14(0)
Koenig_demo_10		
Koenig_demo_10	36(0)	69(0)
Main: Koenig_demo_10	13(0)	14(0)

Model : Koenig_demo_10 (Koenig_demo_10)

L3V1

Koenig Demo Metabolism

Description

This is a demonstration model in SBML format.
The content of this model has been carefully created in a manual research effort.
This file has been produced by Matthias Koenig.

Terms of use

Copyright © 2016 Matthias Koenig.

Redistribution and use of any part of this model, with or without modification, are permitted provided that the following conditions are met:

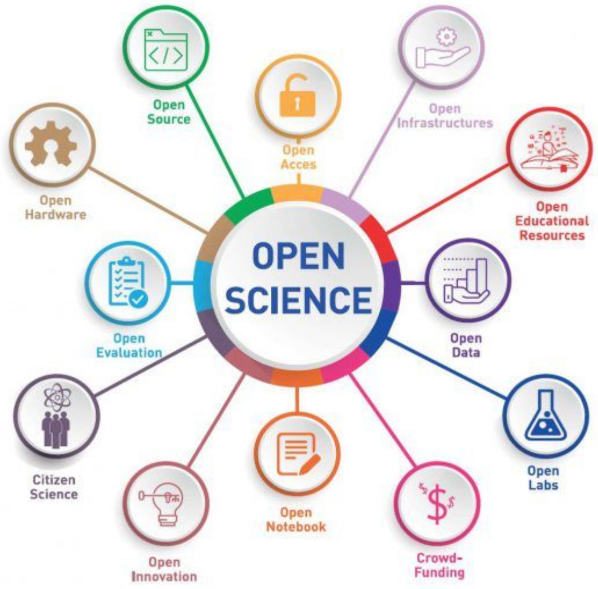
1. Redistributions of this SBML file must retain the above copyright notice, this list of conditions and the following disclaimer.
2. Redistributions in a different form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.

This model is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.

shared name	name	id	sbml-type	sbo	metaId	biomodels.sbo	go	fma	label	value	units	derivedUnits	constant
external compartment	external c...	e	compartment	SBO:0000...	meta_22d897...	SBO:0000290	GO:0005...	FMA:70022	external co...	1.0E-6	m3	m^3	☐
cell compartment	cell comp...	c	compartment	SBO:0000...	meta_78b0e7...	SBO:0000290	GO:0005...	FMA:68646	cell compar...	1.0E-6	m3	m^3	☐
plasma membrane	plasma m...	m	compartment	SBO:0000...	meta_bcdb47...	SBO:0000290	GO:0005...	FMA:63841	plasma me...	1.0	m2	m^2	☐
		Km_C	parameter	SBO:0000...	meta_c63c69...	SBO:0000027			Km_C	3.0	mM	mol*m^(-3)	☑
metabolic scaling fa...	metabolic ...	scale_f	parameter						metabolic s...	1.0E-6	dimensionl...	dimensionless	☑
		Vmax_bB	parameter	SBO:0000...	meta_871a28...	SBO:0000186			Vmax_bB	2.0	mole_per_s	mol*s^(-1)	☑
		Vmax_bC	parameter	SBO:0000...	meta_ad898f...	SBO:0000186			Vmax_bC	2.0	mole_per_s	mol*s^(-1)	☑
		Vmax_bA	parameter	SBO:0000...	meta_351d07...	SBO:0000186			Vmax_bA	5.0	mole_per_s	mol*s^(-1)	☑
		Vmax_v2	parameter	SBO:0000...	meta_074616...	SBO:0000186			Vmax_v2	0.5	mole_per_s	mol*s^(-1)	☑
		Vmax_v3	parameter	SBO:0000...	meta_1e2e9b...	SBO:0000186			Vmax_v3	0.5	mole_per_s	mol*s^(-1)	☑
		Vmax_v1	parameter	SBO:0000...	meta_78fe37...	SBO:0000186			Vmax_v1	1.0	mole_per_s	mol*s^(-1)	☑
		Km_A	parameter	SBO:0000...	meta_98f0e1...	SBO:0000027			Km_A	1.0	mM	mol*m^(-3)	☑
		Vmax_v4	parameter	SBO:0000...	meta_20f045...	SBO:0000186			Vmax_v4	0.5	mole_per_s	mol*s^(-1)	☑

https://github.com/matthiaskoenig/cy3sbml

Open und FAIR Science



FE Kohrs, … , **M König**, …, TL Weissgerber. **Eleven Strategies for Making Reproducible Research and Open Science Training the Norm at Research Institutions.** eLife (2023)

Ten Simple Rules for FAIR Sharing of Experimental and Clinical Data with the Modeling Community. **König M,** Grzegorzewski J, Golebiewski M., Hermjakob H, Hucka M, Olivier B, Keating SM, Nickerson D, Schreiber F, Sheriff R, Waltemath D. Preprints 2021, 2021080303, doi: 10.20944/preprints202108.0303.v2.

FAIR Sharing of Reproducible Models of Epidemic and Pandemic Forecast Ramachandran, K.*; **König, M.***; Scharm, M.; Nguyen, T.V.N.; Hermjakob, H.; Waltemath, D.; Malik Sheriff, R.S. (* equal contribution). Preprints 2022, 2022060137 (doi: 10.20944/preprints202206.0137.v1).

Open Data in Repositories

- BioModels DB, GitHub, Zenodo
- PK-DB

Open/FAIR models

- CC-BY, Zenodo, GitHub, FAIR Indicators

Open Science Initiatives

- Strategy development (Open Science Training at Universities)
- Open Science Ambassador (2024-2025)