

OneStop

JWS Online's access point to SBML, SBGN
and MIRIAM compliant annotation

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& JJJ group for molecular and cellular physiology
Stellenbosch University**

JWS Online

- Among the first online model repositories and simulators

Repository

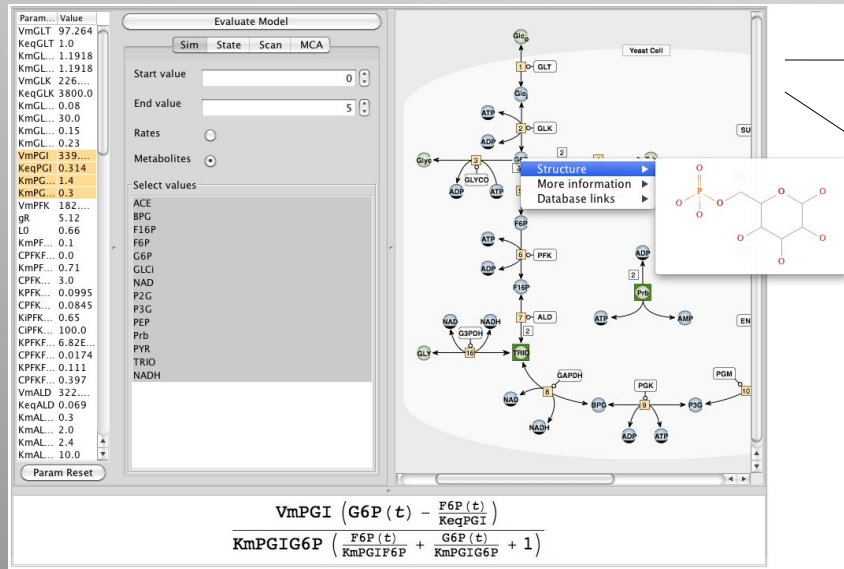
- Review tool for some journals
- 112 curated models
 - Literature
 - Direct communication
(often as part of review process)

+ Simulable copies of BioModels

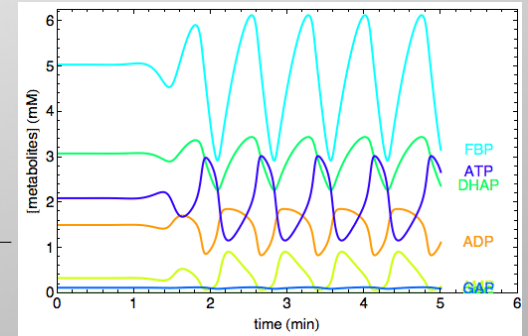
+ Private models for research groups

Simulator

Web based, easy to use interface



Standard simulation functionality



Steady state	[Metabolites] (mM)	Fluxes ((μ M)/(L \cdot min))
ACE	0.170117	v[1] 88.1505
BPG	0.000329694	v[2] 88.1505
F16P	0.801955	v[5] 77.3505
F6P	0.11285	v[3] 6.
G8P	1.03346	v[6] 77.3505
GLCi	0.0987437	v[7] 77.3505
NAD	1.54556	v[16] 18.2025
P2G	0.0448491	v[8] 136.499
P3G	0.35652	v[9] 136.499
PEP	0.0736332	v[10] 136.499
Prb	6.3094	v[11] 136.499
PYR	8.52341	v[12] 136.499
TRIO	0.777558	v[13] 136.499
NADH	0.0444399	v[14] 3.64049
		v[15] 129.218
		v[17] 99.0961

Models can be accessed via web services.
Data linked to models via file upload (e.g. Excel), or via database connection.

SysMO integration

- Used by SysMO consortium
- Systems Biology of Micro-Organisms
 - Generates data for model construction
- SysMO is developing a software platform:
 - **the SEEK**
 - Uses JWS Online as model simulator



the SEEK

- **Aspects**

- **Data capturing**

- **Bottom-up construction data**
 - **Top-down validation data**

- **Model simulation**

- **Social network**

- **Goals**

- **Sharing, Exchange, Reuse, Preservation of modeling research**



*"Find, build, describe and exchange
within Systems Biology"*

www.sysmo-db.org

New needs

Arising from SysMO integration

1.) Provide easy access to modeling standards

OneStop

2.) Facilitate Data integration

DataFuse

Arising from review process

3.) Describe model simulation experiments
(SED-ML)

1.) One Stop to model standards

SBML model format, **SBGN** schema generation, **MIRIAM** annotation

SEEK integrated tool to:

- construct, modify, save models in SBML format
- SBGN schema generation
- annotate model (MIRIAM), using semanticSBML webservice.

The screenshot shows the SEEK web interface. On the left is a sidebar with buttons for 'Simulate', 'Steady State Analysis?' (with a 'Simulate' sub-button), 'Save as new version', 'Model format:' (set to 'SBML'), 'Validate' (with a 'Check' sub-button), and 'Annotator' (with an 'Annotate' sub-button). The main area has a 'Model name' dropdown, a 'Reactions' section with a text area containing:
 $v[v1] \{1.0\}s = \{1.0\}x2$
 $v[v2] \{1.0\}x2 = \{1.0\}x3$
 $v[v3] \{1.0\}x3 = \{1.0\}p$
Below the text area are buttons for 'Reactions help', 'Show schema', and 'Hide schema'. Further down are 'Zoom' and 'Move' controls with directional arrows. At the bottom is a 'Download schema' button. The main visualization is a SBGN diagram showing a reaction network: a source 's' (green circle) leads to 'v1' (yellow circle), which leads to 'x2' (blue circle), which leads to 'v2' (yellow circle). 'v2' leads to 'x3' (blue circle), which leads to 'v3' (yellow circle), which leads to a product 'p' (green circle). There are also labels 'vv1', 'vv2', and 'vv3' above 'v1', 'v2', and 'v3' respectively.



2.) DataFuse

Goal

- Link models to
 - Construction data
 - Validation data

Find, share and exchange **Data, Models and Processes** within the **SysMOOO Testing**.

- People
- Projects
- Institutions
- Investigations
- Studies
- Assays
- Data
- Models
- SOPs
- Publications
- Forums
- Events
- Help

Provide Feedback

 All Go

New or upload

 Go

Announcements

Nature Precedings : doi:10.1038/npre.2011.6349.1.v1

Post announcement 3 months ago by Stuart Owen

Announcements now in SysMO-DB about 1 year ago by Stuart Owen

[See all](#)

Favourites

Drag an icon here to remember for future reference.

Tags [show all]

Bacillus subtilis

Biochemistry

Bioinformatics Computational

and theoretical biology

Computational Systems Biology

Data Management dynamics and

control of biological ne...

Fermentation Genetics

Mathematical modelling

Matlab Microarray analysis

Microbiology

Molecular Biology ODE

parameter estimation Protein

Selected model



cronwright

View
 Download

Creator: Jacky Snoep
Uploader: Jacky Snoep
Model type: Ordinary differential equations
Model format: SBML
Tags: *Not specified*

Version: 1
Associated project: SysMO-LAB
Organism: *Saccharomyces cerevisiae*
Environment: JWS Online

glycerol branch

Created: 08/03/2011 @ 12:27:23 Last updated: 11/04/2011 @ 09:29:51

Selected data file



Cronwright model parameter data

View
 Download
 Manage

Creator: Franco Du Preez
Uploader: Franco Du Preez
Tags: *Not specified*

Version: 6
Associated project: SysMO-DB

No description set

Created: 29/05/2011 @ 13:28:23

Matching parameter symbols and values

ATP	F16BP	Vf1
1.39	8.01	21.0
3.56	3.96	80.0



Provide Feedback

Search bar with dropdown menu and Go button

New or upload
Data file [] Go

Announcements
test announcement 3 months ago by Stuart Owen.
Announcements now in Sysmo-SEEK about 1 year ago by Stuart Owen
See all

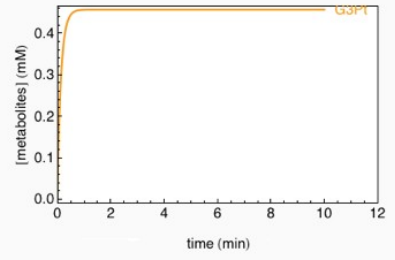
Favourites
Drag an icon here to remember for future reference.

Tags [show all]
Bacillus subtilis
Biochemistry
Bioinformatics Computational and theoretical biology
Computational Systems Biology
Data Management dynamics and control of biological ne...
Fermentation Genetics
Mathematical modelling
Matlab Microarray analysis
Microbiology
Molecular Biology ODE
parameter estimation Protein analysis SBML Systems Biology
Transcriptomics

Organisms
Bacillus subtilis
Chimpanzee papillomavirus
Clostridium acetobutylicum
Enterococcus faecalis
Escherichia coli
Hoplopsyllus anomalus
Lactic Acid Bacteria
Lactococcus lactis
Mus
Mus abboti
Mus musculus
Pseudomonas fluorescens
Pseudomonas putida
Saccharomyces cerevisiae
Streptococcus pyogenes
Streptomyces coelicolor
Sulfolobus solfataricus

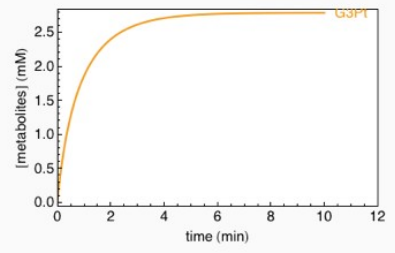
simWithOrigParams

Download as CSV | View Results



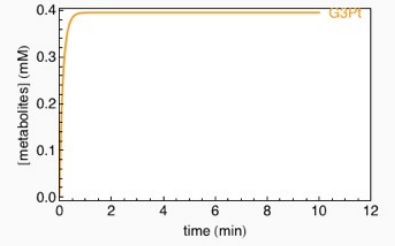
simWithExpParams1

Download as CSV | View Results



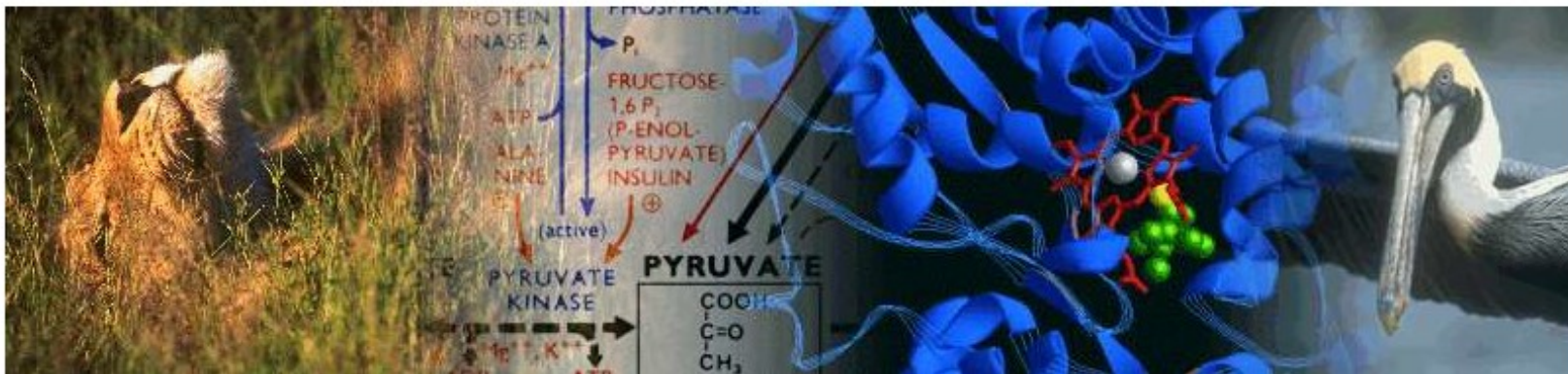
simWithExpParams2

Download as CSV | View Results



3.) Describe model simulation experiments (SED-ML)

- To recreate published tables and figures
 - for curated models
 - for models being reviewed
 - (to replace customized Mathematica packages for each model)
- To automate modeling workflows for users



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SED-ML support

Enter SED-ML file:

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<sedml:sedML xmlns:sedml="http://sed-ml.org" xmlns:math="http://www.w3.org/1998/Math/MathML">
  <sedml:listOfModels>
    <sedml:model id="model1" name="bier" source="urn:miriam:jws:bier" language="urn:sedml:language:jwsonlinepackage" >
      </sedml:model>
    <sedml:model id="model2" name="bierPerturbed" source="urn:miriam:jws:bier" type="jwspackage">

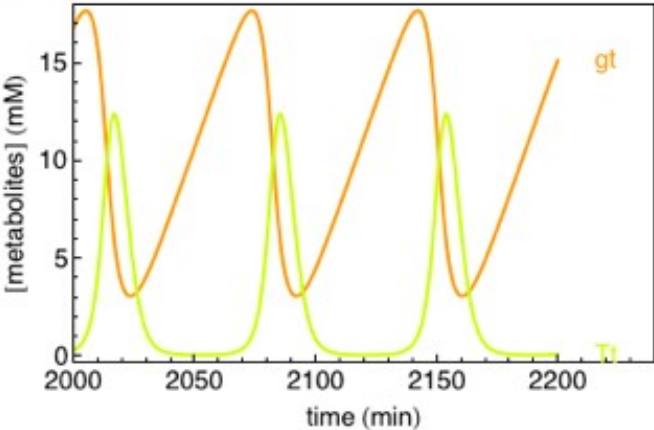
```

no file selected

SED-ML simulation results:

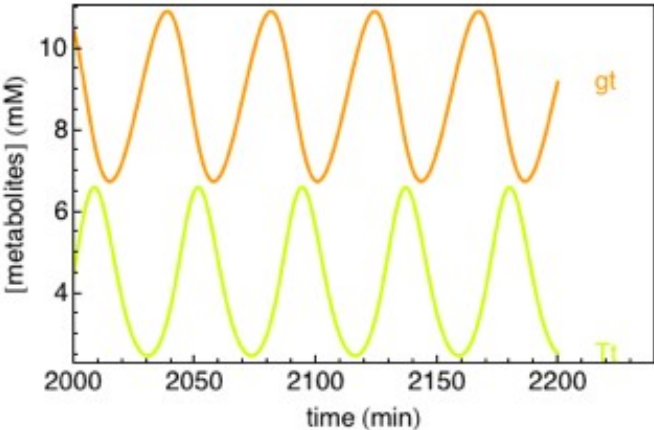
Task: simulatebier

Model: bier



Task: simulatebierPerturbed

Model: bierPerturbed



Acknowledgements

- SysMO-DB team
 - Carole Goble (FBCS Manchester)
 - Stuart Owen
 - Katy Wolstencroft
 - Wolfgang Mueller (HITS)
 - Jacky Snoep (Stellenbosch)
- Funding: This work was funded by the BBSRC and the BMBF. SysMO-DB: Supporting Data Access and Integration (BBG0102181).