

# OneStop

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

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# JWS Online

- Among the first model repositories and simulators

## **Repository**

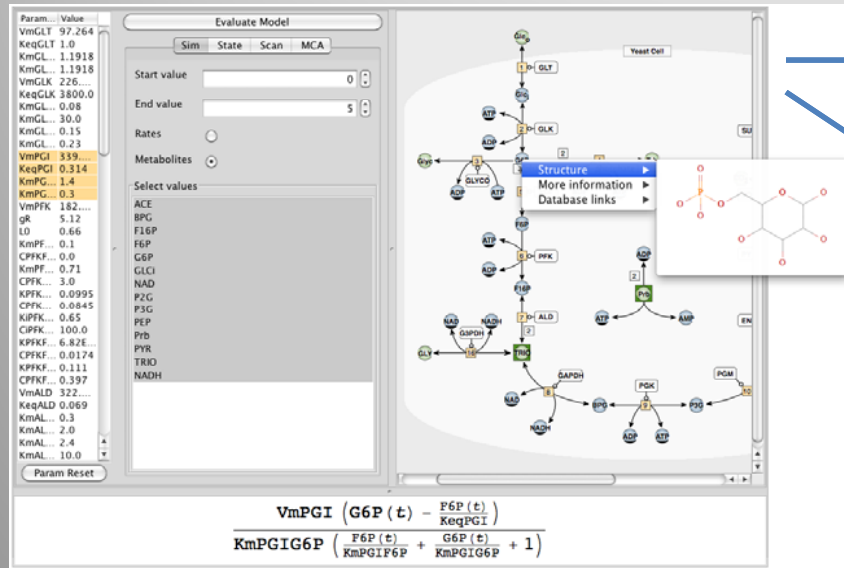
- Review tool for some journals
- 112 curated models
  - Literature
  - Direct communication  
(often as part of review process)

+ Simulable copies of Biomodels

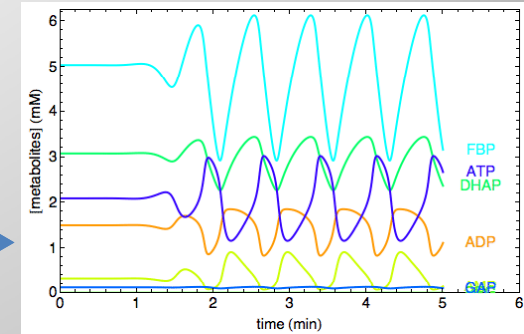
+ Private models for some research groups

# Simulator

Web based, easy to use interface



Standard simulation functionality

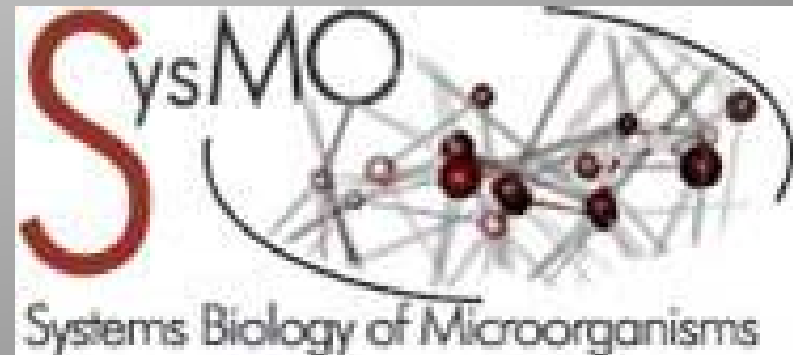


Steady state			
	[Metabolites] (mM)		Fluxes (( $\mu$ M)/(L $\cdot$ min))
		v[1]	88.1505
		v[2]	88.1505
ACE	0.170117	v[5]	77.3505
BPG	0.000329694	v[3]	6.
F16P	0.801955	v[4]	2.4
F6P	0.11285	v[6]	77.3505
G6P	1.03346	v[7]	77.3505
GLCi	0.0987437	v[16]	18.2025
NAD	1.54556	v[8]	136.499
P2G	0.0448491	v[9]	136.499
P3G	0.35652	v[10]	136.499
PEP	0.0736332	v[11]	136.499
Prb	6.3094	v[12]	136.499
PYR	8.52341	v[13]	136.499
TRIO	0.777558	v[14]	3.64049
NADH	0.0444399	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](http://www.sysmo-db.org)**

# New goals

## 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

The screenshot shows the SEEK software interface. On the left is a sidebar with buttons for 'Simulate', 'Steady State Analysis?' (with a 'Simulate' button), 'Save as new version', 'Model format:' (set to 'SBML'), 'Validate' (with a 'Check' button), and 'Annotator' (with an 'Annotate' button). The main area has a 'Model name' dropdown, a 'Reactions' dropdown, and a text box containing the following SBML reaction definitions:

```
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 box are buttons for 'Reactions help', 'Show schema', and 'Hide schema'. There are also 'Zoom' and 'Move' controls with directional arrows. At the bottom of the main area is a 'Download schema' button. The bottom part of the interface displays a SBGN diagram with nodes labeled v1, v2, v3, s, and p, and reactions x2 and x3.

SEEK integrated tool to:

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



## 2.) DataFuse

### Goal

- Link models to
  - Construction data
  - Validation data





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

Logged in as Franco Du Preez | Logout



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

Provide Feedback

 All 

New or upload

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

### 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

New or upload

Data file

**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]**

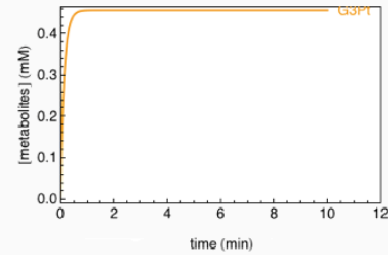
- Bacillus subtilis
- Biochemistry**
- Bioinformatics Computational and theoretical biology
- Computational Systems Biology
- Data Management dynamics and control of biological ne...
- Fermentation Genetics
- Mathematical modelling
- Matlab Microarray analysis
- Microbiology**
- Molecular Biology ODE**
- 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 abbotti
- Mus musculus
- Pseudomonas fluorescens**
- Pseudomonas putida
- Saccharomyces cerevisiae
- Streptococcus pyogenes
- Streptomyces coelicolor
- Sulfolobus solfataricus

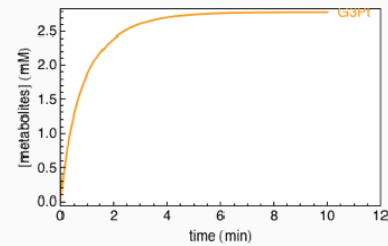
**simWithOrigParams**

[Download as CSV](#) | [View Results](#)



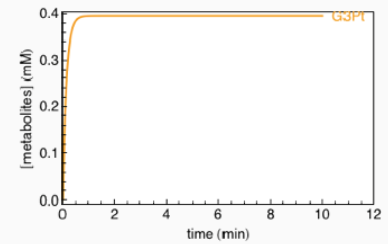
**simWithExpParams1**

[Download as CSV](#) | [View Results](#)



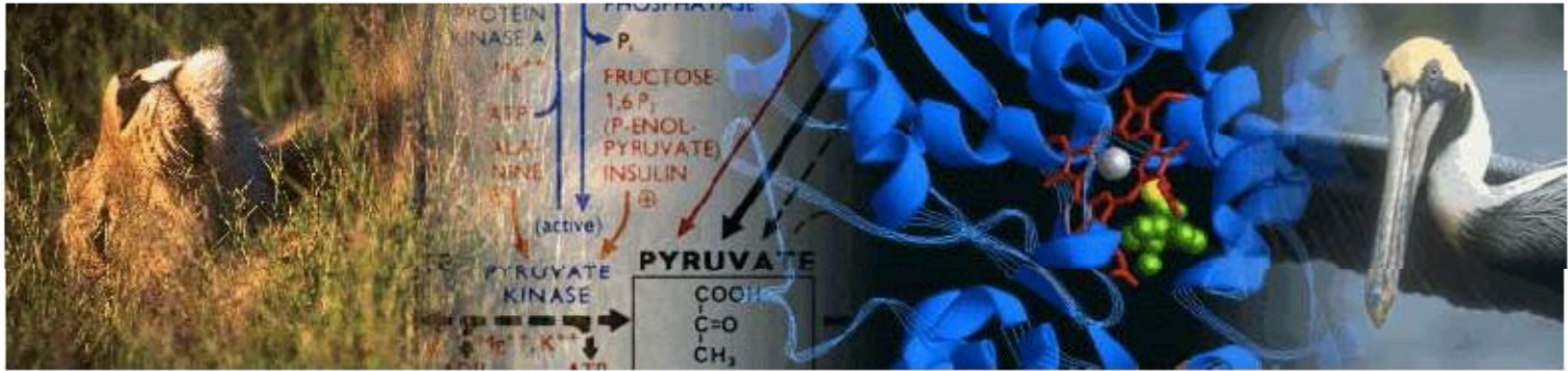
**simWithExpParams2**

[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



## SED-ML support

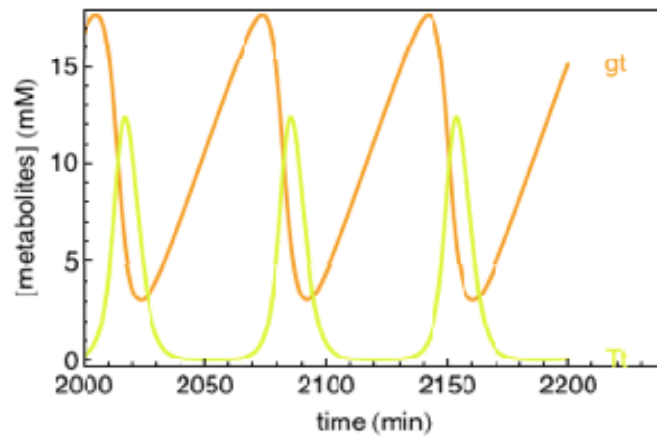
Enter SED-ML file:

```
<?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">
      </sedml:model>
    </sedml:listOfModels>
  </sedml:sedML>
```

## SED-ML simulation results:

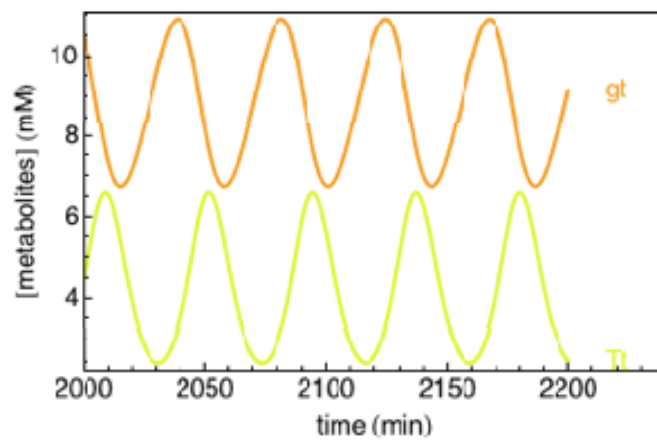
**Task: simulatebier**

**Model: bier**



**Task: simulatebierPerturbed**

**Model: bierPerturbed**



# Acknowledgements

- SysMO-DB team
  - Carole Goble (FBCS Manchester)
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  - 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).







# SEEK Facts and Figures

## Registered Users: 325 (202)

- 21,600 page views, 520 unique visitors, 110 unique users log ins.
- User visits: >30% at least once per week, > 50% at least once per month

## Registered Content:

- Investigations 24 (19) | Studies 64 (46) | Assays 127 (99)
  - Data files 862 (590)
  - Models 33 (23)
  - SOPs 119 (116)
  - Publications 109 (37)
- > 15 JERMs



# Modelling standards

	Models	Simulations	Results
<b>Minimum information models</b>	MIRIAM <sup>[1]</sup>	MIASE	
<b>Standard formats</b>	SBML <sup>[1]</sup> , Human readable JWS Online format <sup>[1]</sup>	SED-ML	SBRML
<b>Ontologies and nomenclatures</b>	Chebi, KEGG, EC numbers etc accessed as MIRIAM URIs via SemanticSBML <sup>[1]</sup>	KISAO	TEDDY
<b>Databases</b>	BioModels, JWS Online		
<b>Graphic notation</b>	SBGN <sup>[1]</sup>		

1. Implemented in JWS Online











