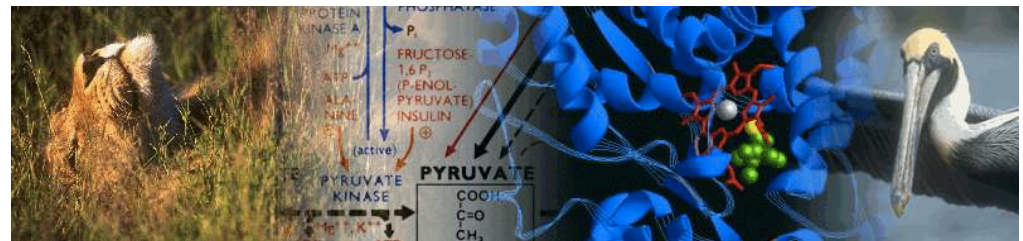


# The new JWS Online simulation interface: SBGN schema generation, MIRIAM annotation and SBML model specification

Franco du Preez, Jacky L Snoep and SysMO-DB team:  
Olga Krebs, Katy Wolstencroft, Stuart Owen, Lihua An, Martin  
Golebiewski, Quyen Nguyen, David Shockley, Andreas Weidemann,  
Carole Goble, Wolfgang Müller

Manchester Institute for Biotechnology, University of Manchester  
& JJJ group for molecular and cellular physiology  
Stellenbosch University



# Outline

- 1.) What is JWS Online?
- 2.) JWS Online components
- 3.) Demonstration of new simulator
- 4.) Linking models and data

# JWS Online

- Among the first online model repositories and simulators

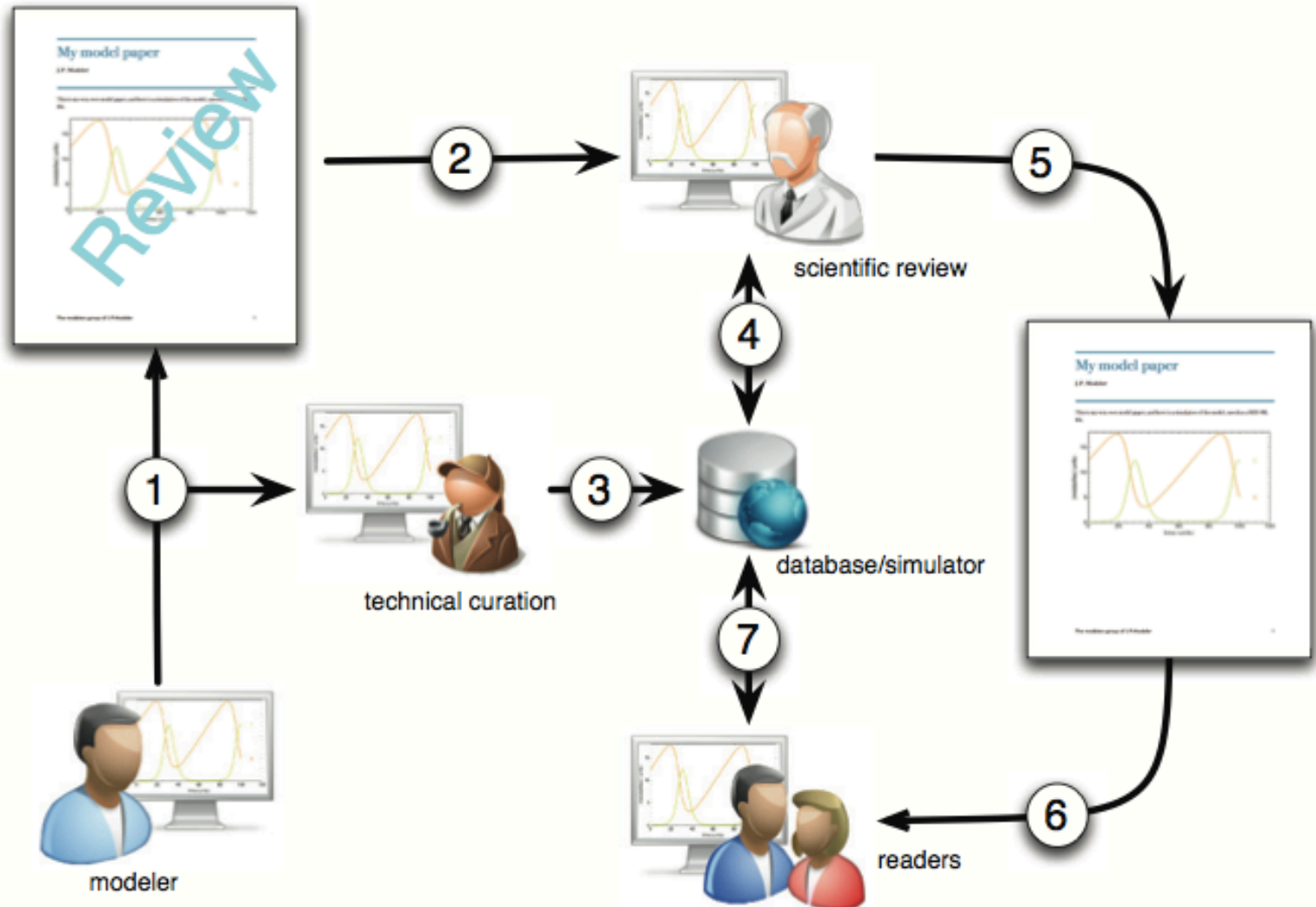
## **Repository**

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

+ Simulable copies of BioModels

+ Private models for research groups

# JWS Online Model curation



# SysMO integration

- Used by SysMO consortium
- Systems Biology of Micro-Organisms
  - Generates data for model construction
- SysMO develops 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)**

# JWS Online components

Human readable  
model format

**Simulate**

☐ Steady State Analysis?  
**Simulate**

**Save as new version**

Model format:  
SBML   
**Save**

**Validate**

**Check**

**Annotator**

**Annotate**

create  
edit

export  
view

SBML

Model name

**Reactions**

```
v[v1] {1.0}$s = {1.0}x2  
v[v2] {1.0}x2 = {1.0}x3  
v[v3] {1.0}x3 = {1.0}$p
```

Reactions help Show schema Hide schema

Zoom Move

+ - ← → ↑ ↓

Download schema

SBGN-ML

SBGN  
schema

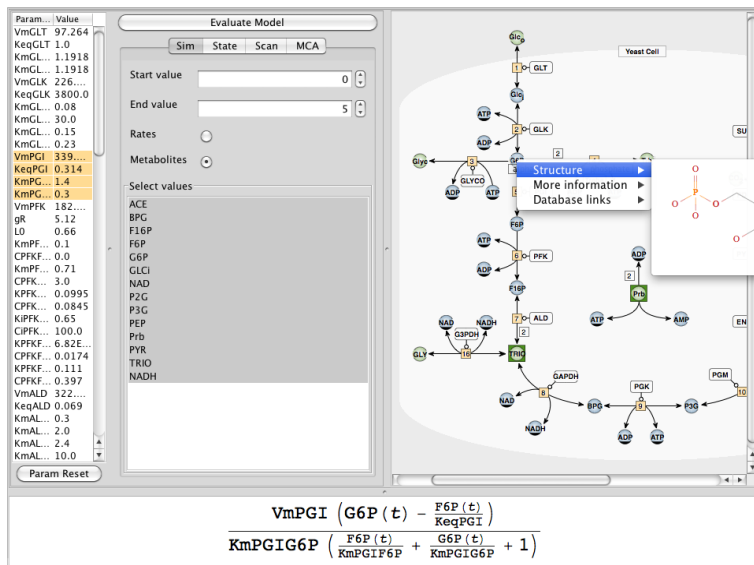
MIRIAM  
annotated  
components

SED-ML

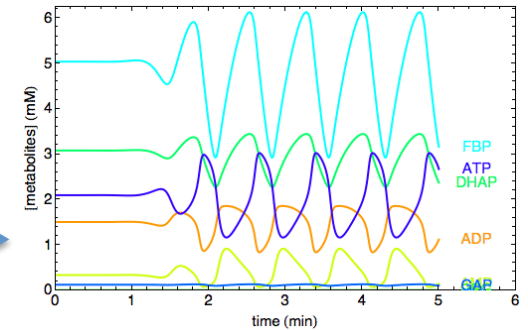
Stoichiometric  
matrices

# Simulator

Web based, easy to use interface



Standard  
simulation  
functionality



Steady state

	[Metabolites] (mM)		Fluxes ((cyt*mM)/(L*min))
ACE	0.170117	v[1]	88.1505
BPG	0.000329694	v[2]	88.1505
F16P	0.801955	v[3]	77.3505
F6P	0.11285	v[4]	6.
G6P	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



# Simulator upgrade

- **HTML**

mobile friendly

- **Java Applet**

security prompts

loading time

- **SVG**

zoom and pan

link to elements

- **GIF image**

link to coordinates

- **Tabbed results**

- **Pop-up window**

# Upload biomodel


▼ parameters

Name	Value
gR	5.12
KmPFKF6P	0.1
KmPFKATP	0.71
Lzero	0.66
CiPFKATP	100
KIPFKATP	0.65
CPFKAMP	0.0845
KPFKAMP	0.0995
CPFKF26BP	0.0174
KPFKF26BP	0.000682

external variables

initial conditions

Schema



Evaluate model

Sim

State

MCA

Scan

Fun

Enter time period for plotting

Start  End

Save as SED-ML script

Select category to be plotted

Species

Rates

Other

Select species to be plotted

all

none

ACE  
BPG  
F16P  
F6P

Species

GL

I

Go

FO

F1

NA

TR

BE

P3

P2

PI

PY

AC

NA

CPFKA

## Attribution annotation

Model Name:

Citation URL:

Model URN:

### Model creators:

Given name(s):

Surname:

Email:

Institution:

[Add author](#)

Creation

Creat

Mo

Modific

Tern

webMathematica <JLink> org.sbgn.jar

```
<map>  
  <glyph id="glyph9" class="macromolecule">  
    <label text="vGLK"/>  
    <bbox y="360.82" x="349.018" h="9.65455" w="18.0"/>  
  </glyph>  
  ...  
  ...  
  ...  
</map>
```

# Create an error in the SBML and re-upload

```
<apply>  
  <plus/>  
  <cn type="integer"> 1 </cn>  
<apply>  
  <divide/>  
  <ci> F6 </ci>  
  <ci> undefinedElement </ci>  
</apply>
```

# Upload altered model, OneStop outlines error


parameters

Name	Value
gR	5.12
KmPFKF6P	0.1
KmPFKATP	0.71
Lzero	0.66
CiPFKATP	100
KIPFKATP	0.65
CPFKAMP	0.0845
KPFKAMP	0.0995
CPFKF26BP	0.0174
KPFKF26BP	0.000682

external variables

initial conditions

Schema



Evaluate model

Sim

State

MCA

Scan

Fun

Enter time period for plotting

Start  End

Save as SED-ML script

Select category to be plotted

Species

Rates

Other

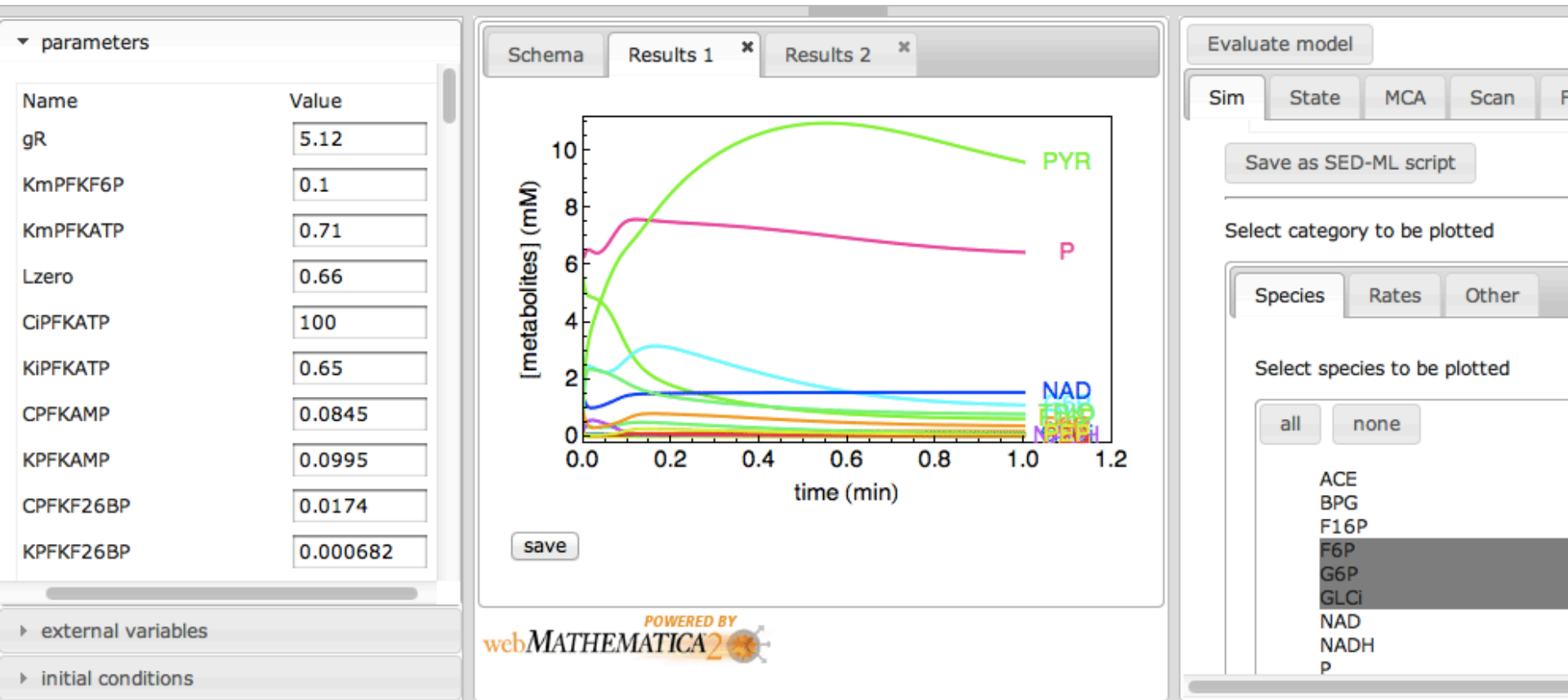
Select species to be plotted

all

none

ACE  
BPG  
F16P  
F6P

# Simulation & analysis

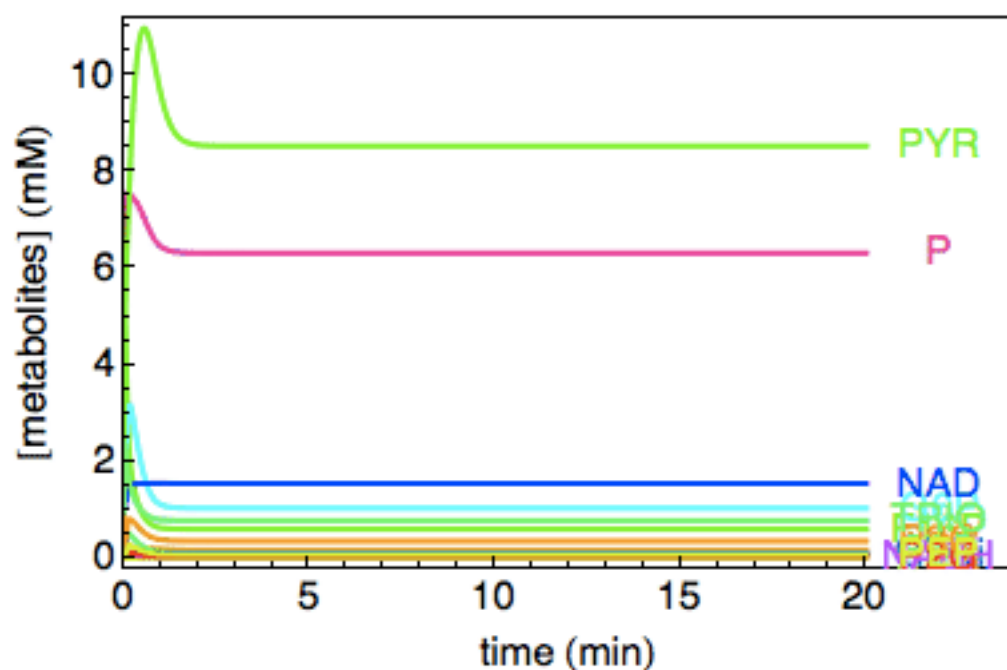


# Export of SED-ML script

## SED-ML simulation results:

Task: simulatebiomodel

Model: teusink



# DataFuse

## Goal

- Link models to
  - Construction data
  - Validation data





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



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[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**

**Creator:** [Jacky Snoep](#)

**Uploader:** [Jacky Snoep](#)

**Model type:** Ordinary differential equations

**Model format:** SBML

**Tags:** *Not specified*

glycerol branch

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

**Version:** 1

**Associated project:** [SysMO-LAB](#)

**Organism:** [Saccharomyces cerevisiae](#)

**Environment:** JWS Online

[View](#)

[Download](#)

### Selected data file



**Cronwright model parameter data**

**Creator:** [Franco Du Preez](#)

**Uploader:** [Franco Du Preez](#)

**Tags:** *Not specified*

No description set

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

**Version:** 6

**Associated project:** [SysMO-DB](#)



[View](#)

[Download](#)

[Manage](#)

### Matching parameter symbols and values

ATP	F16BP	Vf1
1.39	8.01	21.0
3.56	3.96	80.0



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[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

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**Favourites**

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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

Hoplopyllus anomalus

Lactic Acid Bacteria

Lactococcus lactis

Mus

Mus abboti

Mus musculus

Pseudomonas fluorescens

Pseudomonas putida

Saccharomyces cerevisiae

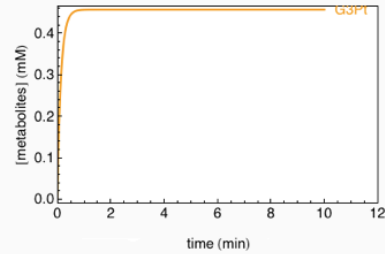
Streptococcus pyogenes

Streptomyces coelicolor

Sulfolobus solfataricus

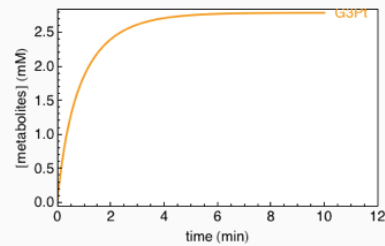
**simWithOrigParams**

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



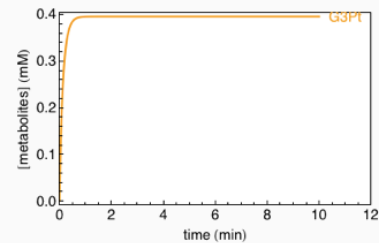
**simWithExpParams1**

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

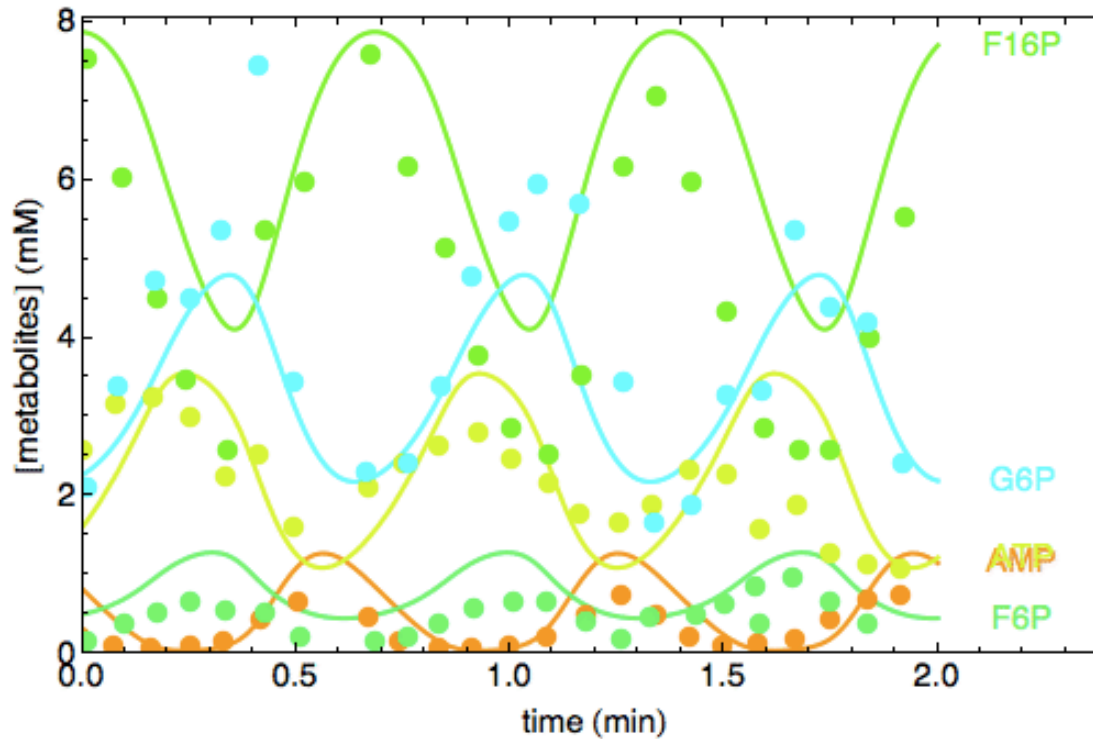


**simWithExpParams2**

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



# Validation data



Download the results in text or comma separated value format (e.g. for Excel import):

Upload data:  no file selected

# Acknowledgements

- SysMO-DB team
  - Carole Goble (FBCS Manchester)
  - Stuart Owen
  - Katy Wolstencroft
  - Wolfgang Mueller (HITS)
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