Applying the Scientific Method to Simulation Experiments

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Scientific Method

Scientific method *– body of techniques for investigating* ***phenomena*** *and acquiring new* ***knowledge****, as well as for* ***correcting and integrating*** *previous knowledge.*

http://en.wikipedia.org/wiki/Scientific_method

Models

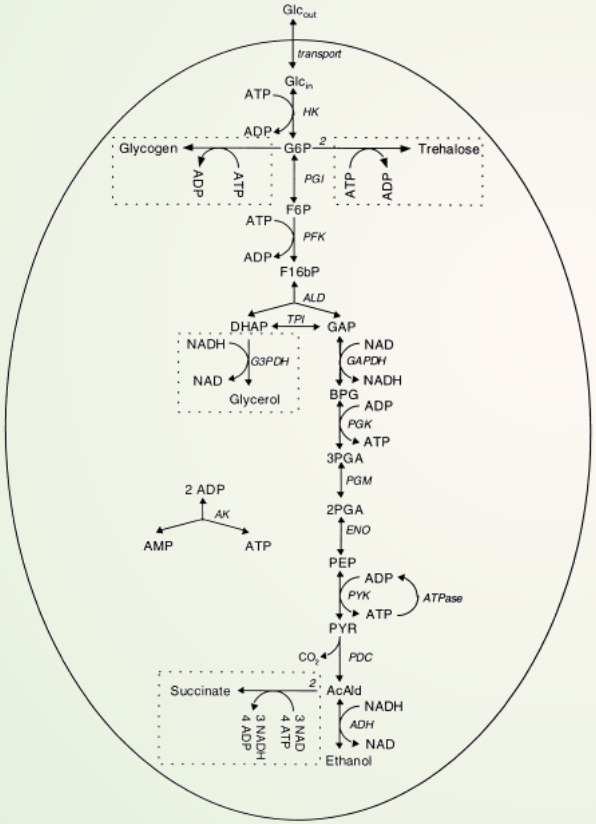


Fig. 1. **Scheme of the model.** Reactions in boxes show the branches introduced in the extended model. GAP, Gra*P*; DHAP, glycerone phosphate; BPG, 1,3GriP_2; 3PGA, 3Gri*P*; 2PGA, 2Gri*P*; PEP, phospho-enol-pyruvate; GAPDH, GraPDH.

$$d[Glc_{in}]/dt = v_{transport} - v_{HK} \quad (6)$$

$$d[G6P]/dt = v_{HK} - v_{PGI} - 2v_{trehalose} - v_{glycogen}) \quad (7)$$

$$d[F6P]/dt = v_{PGI} - v_{PFK} \quad (8)$$

$$d[F1,6bP_2]/dt = v_{PFK} - v_{ALD} \quad (9)$$

$$d[Trio-P]/dt = 2v_{ALD} - v_{GraPDH}\ (-v_{glycerol}) \quad (10)$$

$$d[BPG]/dt = v_{GraPDH} - v_{PGK} \quad (11)$$

$$d[3GriP]/dt = v_{PGK} - v_{PGM} \quad (12)$$

$$d[2GriP]/dt = v_{PGM} - v_{ENO} \quad (13)$$

$$d[phospho\textit{enol}pyruvate]/dt = v_{ENO} - v_{PYK} \quad (14)$$

$$d[PYR]/dt = v_{PYK} - v_{PDC} \quad (15)$$

$$d[AcAld]/dt = v_{PDC} - v_{ADH}\ (-2v_{succinate}) \quad (16)$$

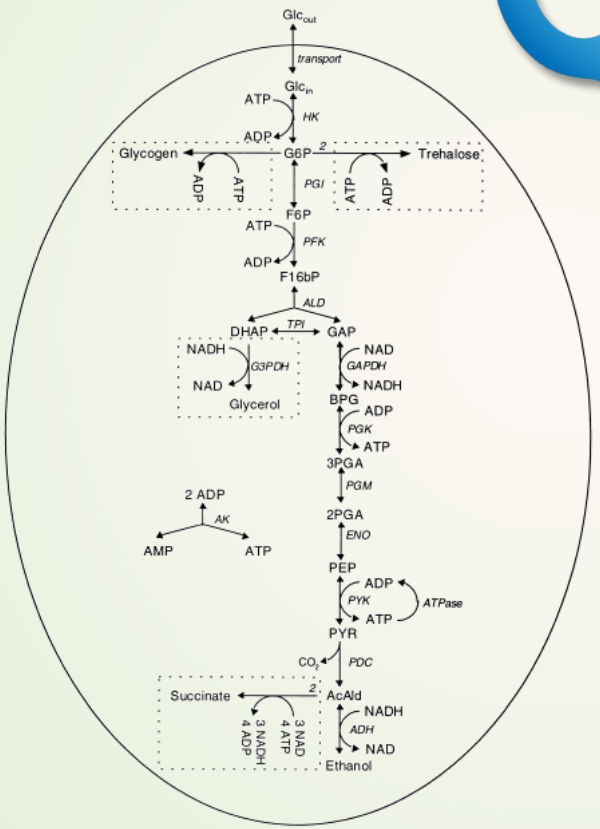
$$dP/dt = -v_{HK} - v_{PFK} + v_{PGK} + v_{PYK} - v_{ATPase}$$
$$(-v_{trehalose} - v_{glycogen} - 4v_{succinate}) \quad (17)$$

$$d[NADH]/dt = v_{GraPDH} - v_{ADH}\ (-v_{glycerol} + 3v_{succinate}) \quad (18)$$

$$d[NAD]/dt = -d[NADH]/dt \quad (19)$$

Teusink et. al, 2003, DOI: 10.1046/j.1432-1327.2000.01527.x

Models



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$$d[\mathrm{Glc}_{in}]/dt = v_{transport} - v_{HK} \quad (6)$$

$$dt = \quad - v_{PGI} - 2v_{trehalose} \quad (7)$$

$$[F6P]/dt = v_{PGI} \quad (8)$$

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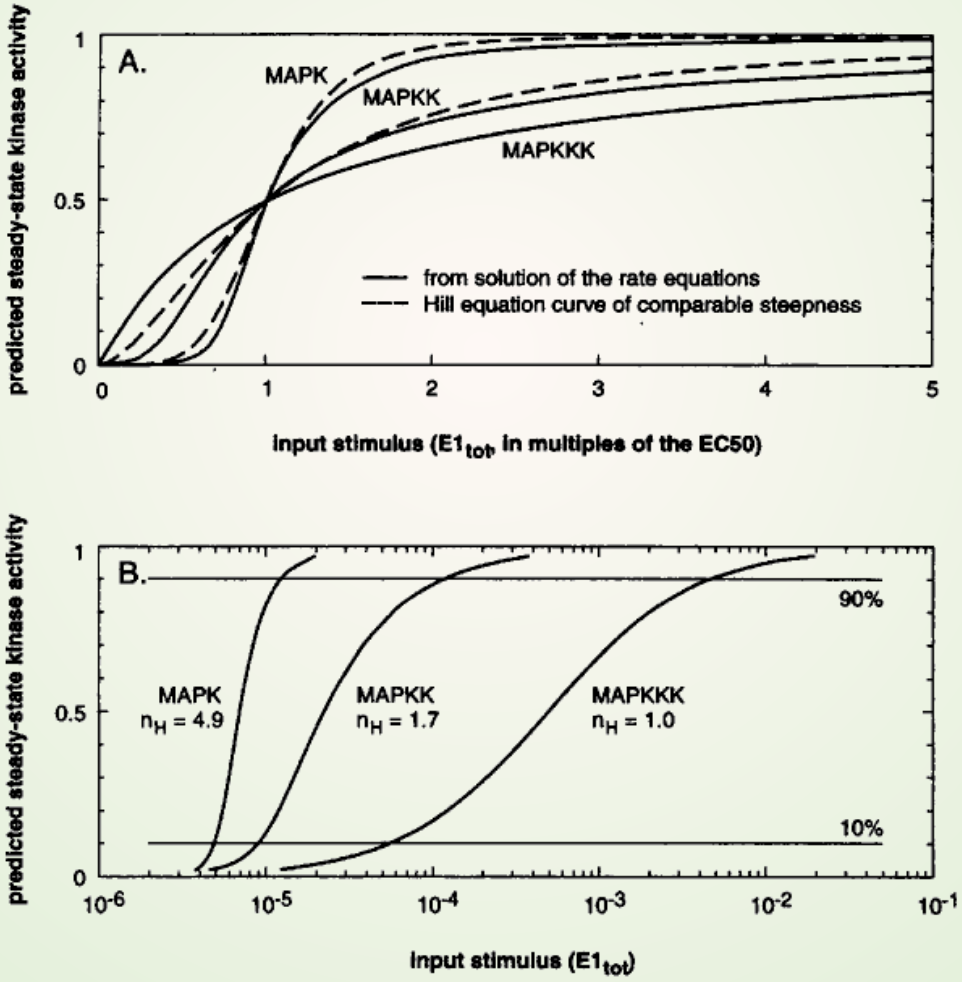
Simulation Experiments



Huang et. al, 1996, DOI: 10.1073/pnas.93.19.10078

Simulation Experiments

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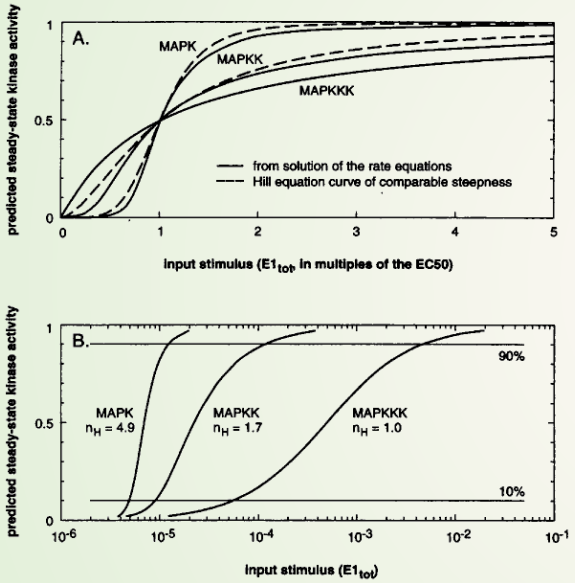

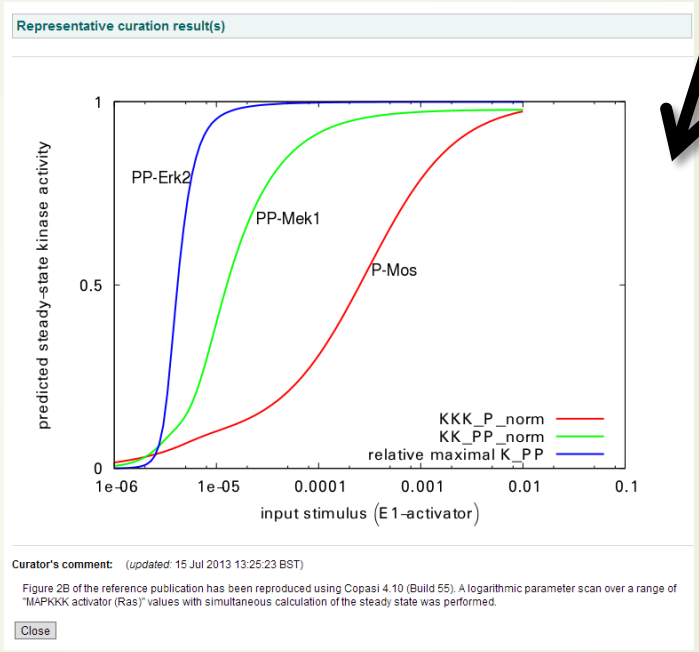

Curator's comment: (*updated:* 15 Jul 2013 13:25:23 BST)
Figure 2B of the reference publication has been reproduced using Copasi 4.10 (Build 55). A logarithmic parameter scan over a range of "MAPKKK activator (Ras)" values with simultaneous calculation of the steady state was performed.

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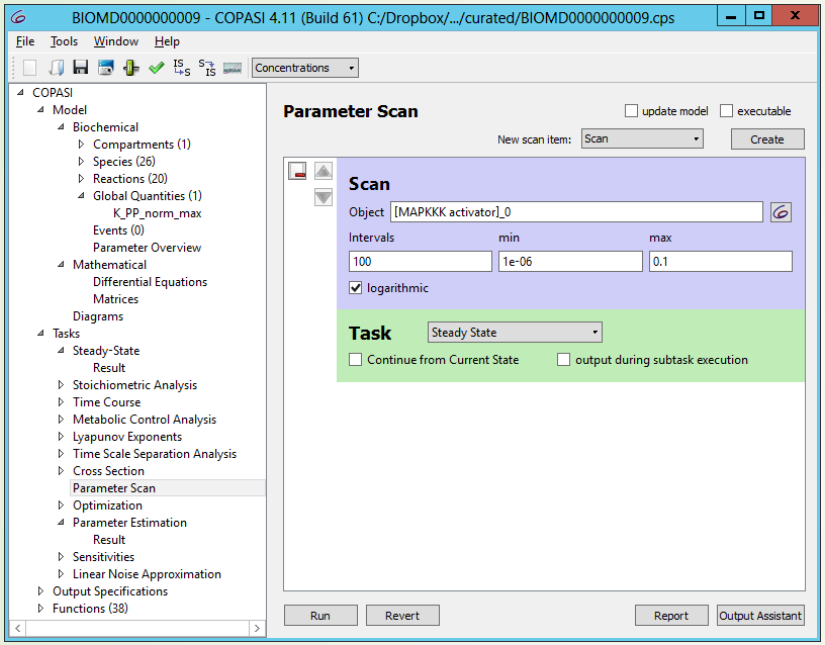
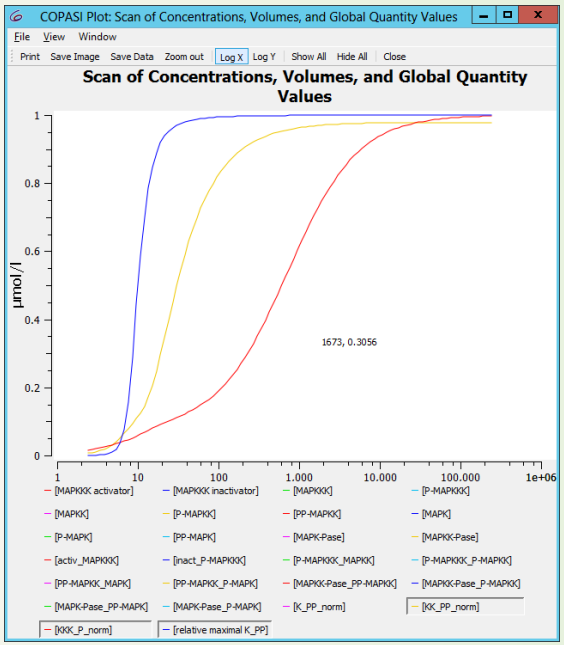
Simulation Experiments





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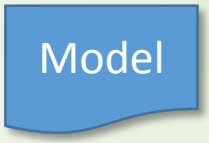
Simulation Experiment Description Markup Language

SED-ML: Repeatable simulation experiments



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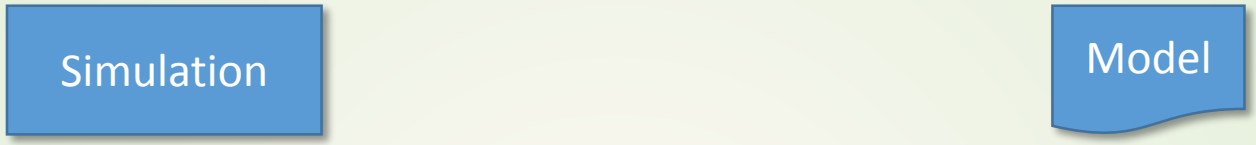

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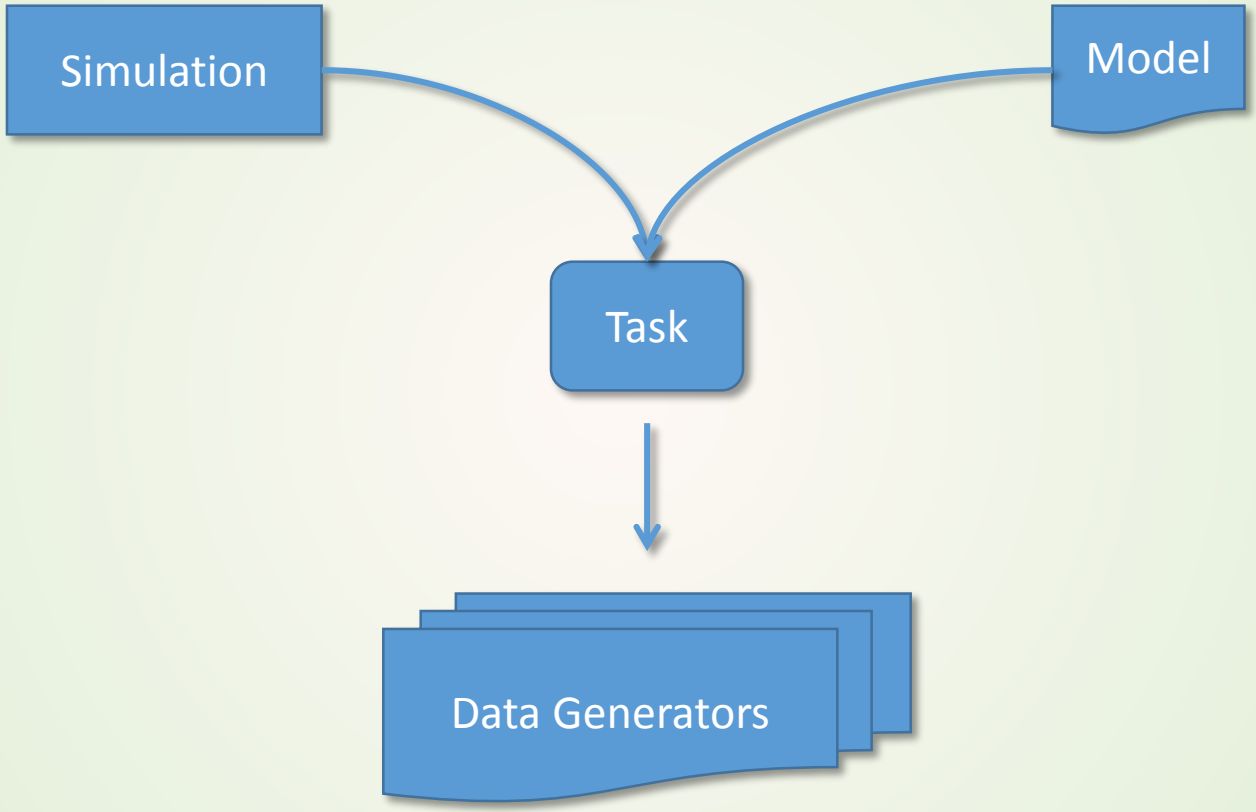
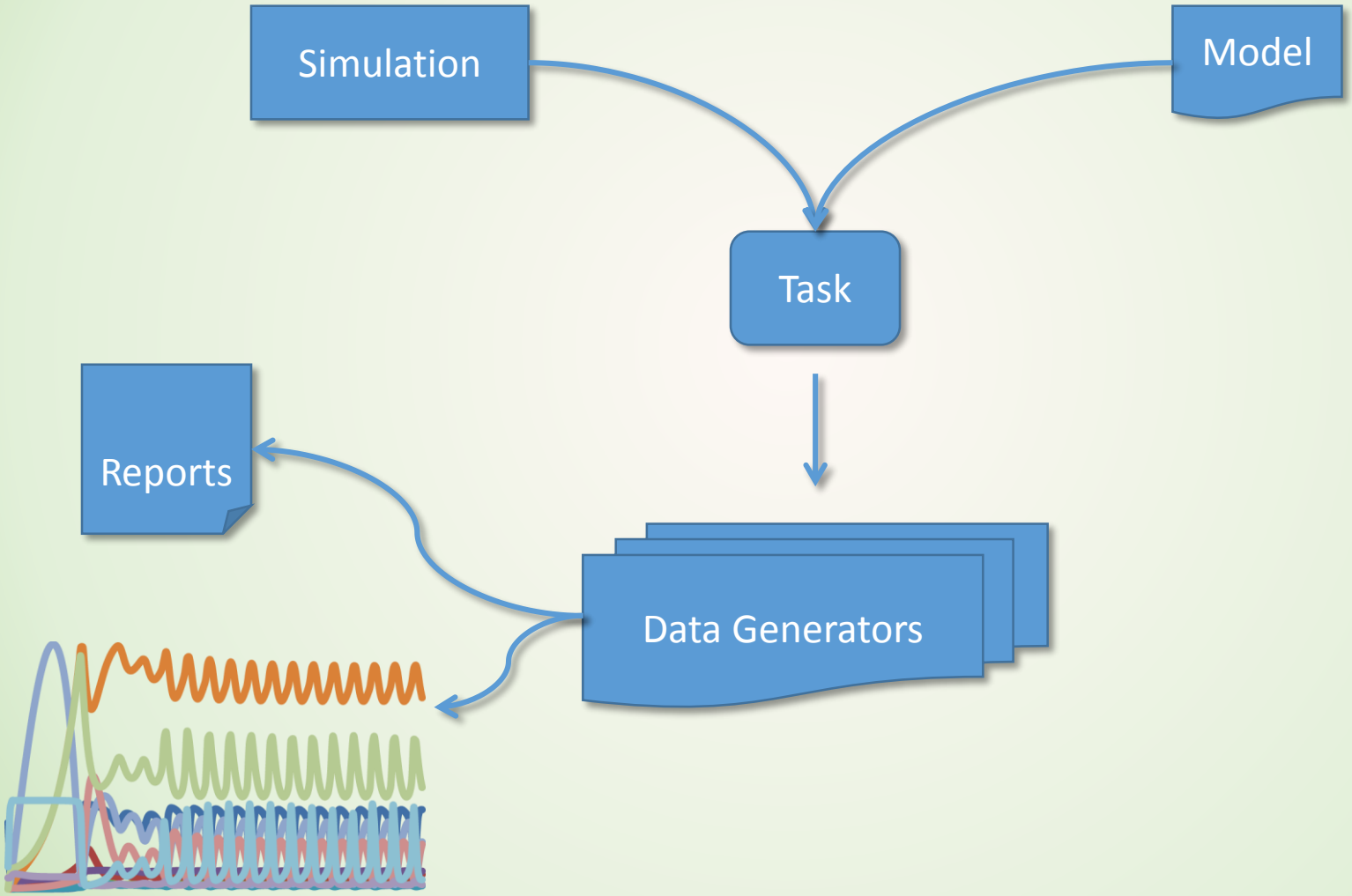


SED-ML: Repeatable simulation experiments



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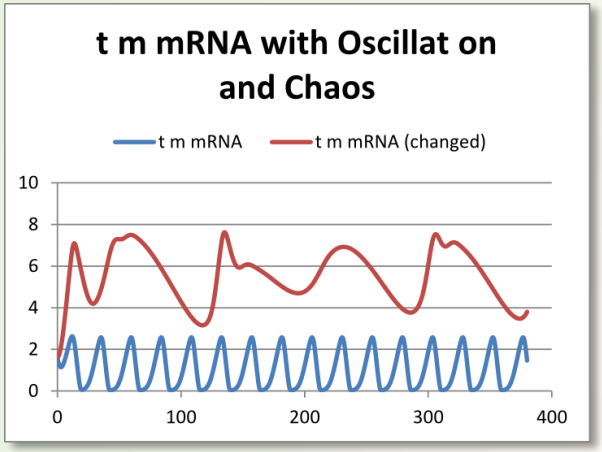
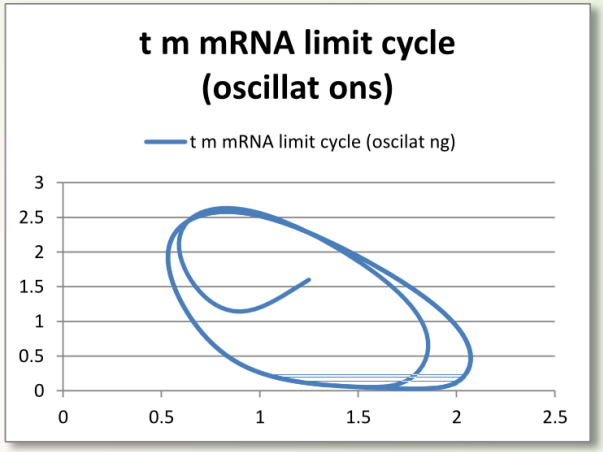
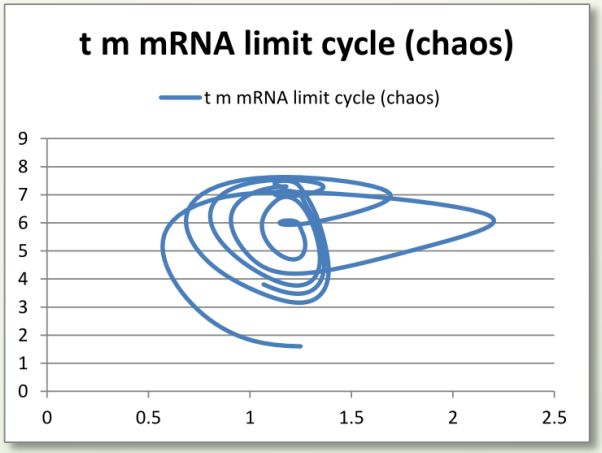
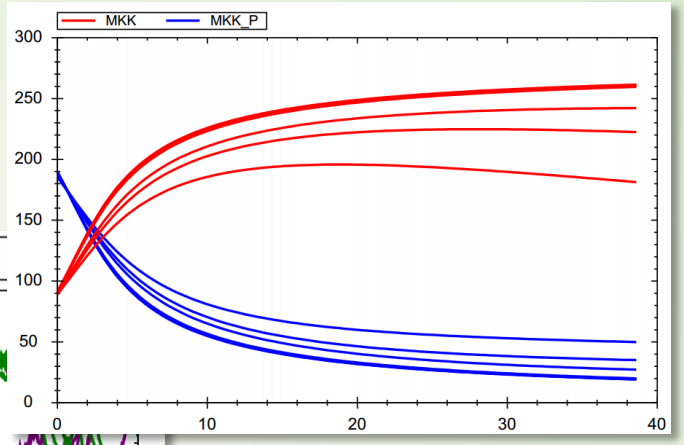






SED-ML L1V2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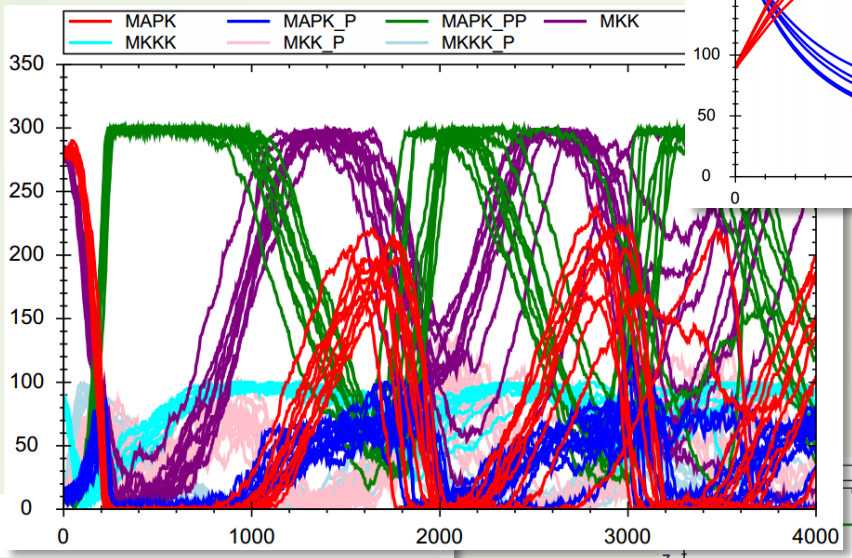
40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MAPK_P
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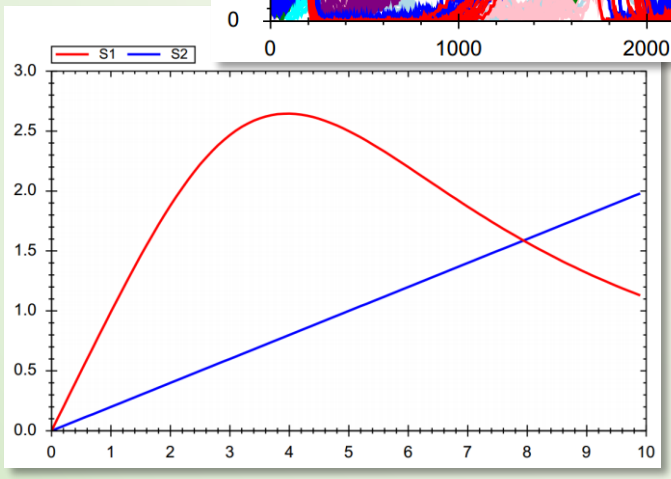
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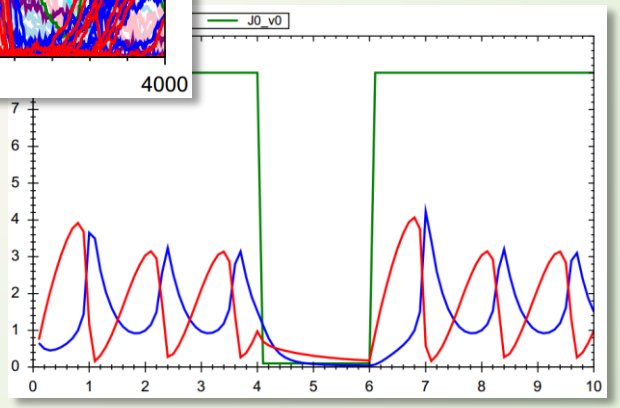
J0_v0
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6
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9
10

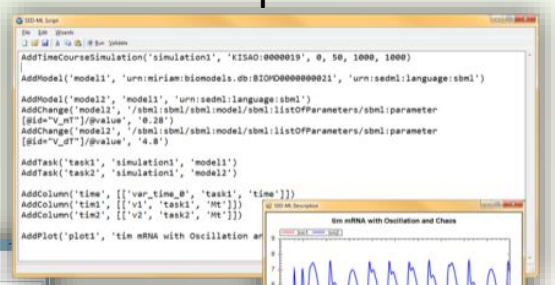
Software Support - Libraries

- libSedML: *.NET*; BSD License
  http://libsedml.sourceforge.net
- libSEDML: *C/C++ with bindings for .NET, Java, Perl, Python, R, Ruby*; BSD License, https://github.com/fbergmann/libsedml

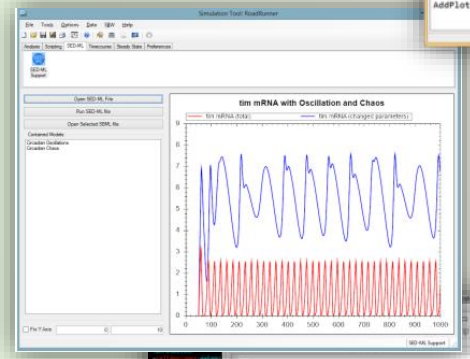
- jlibsedml: *Java*; MIT License
  http://sourceforge.net/projects/jlibsedml/
- clibsedml,: *C*; BSD License
  http://sourceforge.net/projects/clibsedml

Software Support

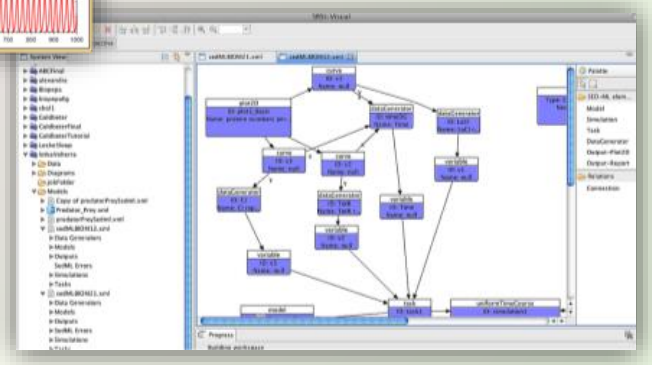
SED-ML Script Editor

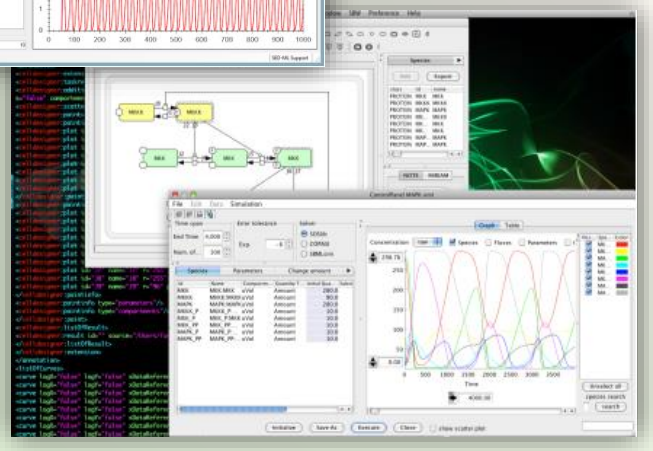


SBW

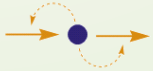


SBSI SED-ED





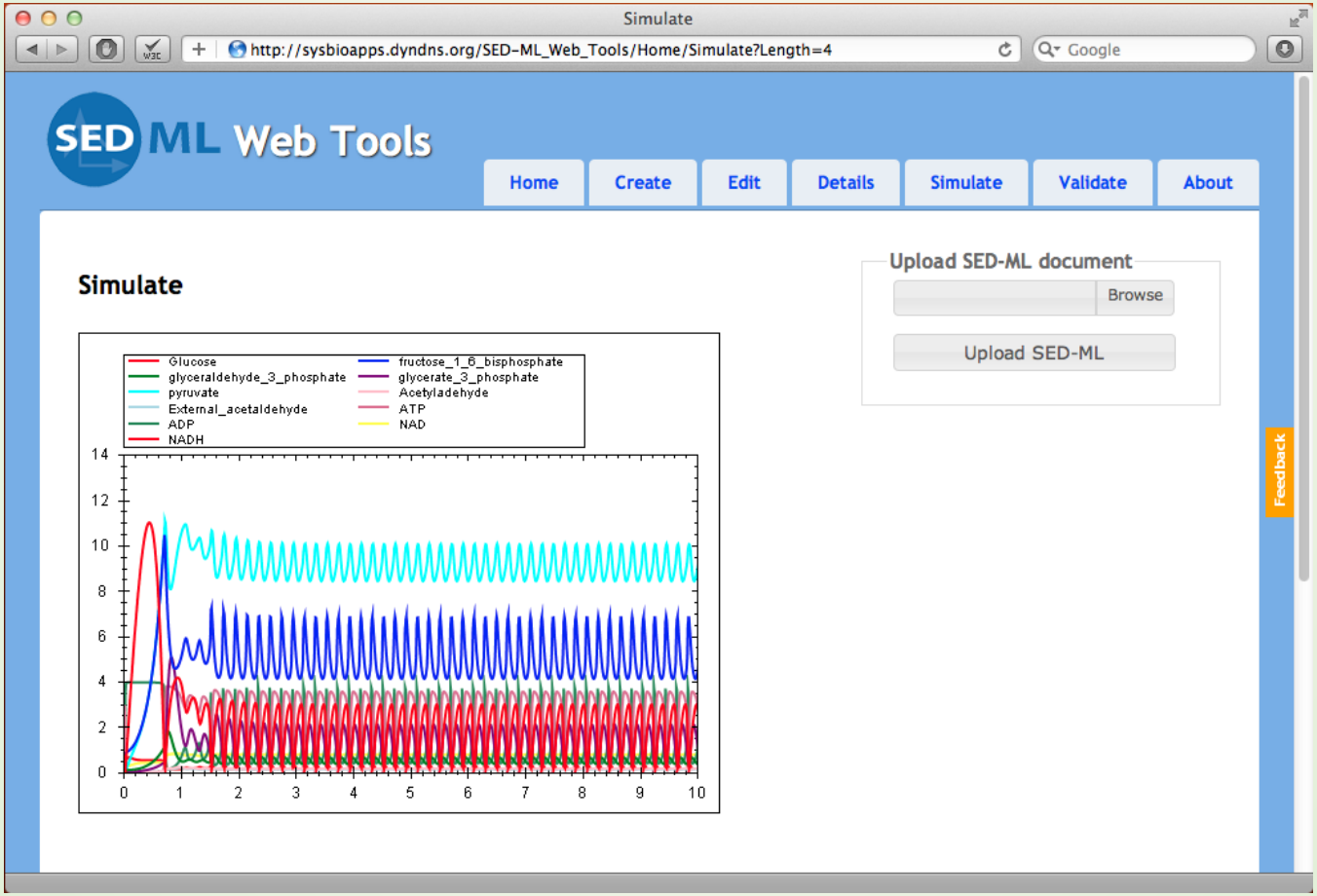
CellDesigner



PySCeS

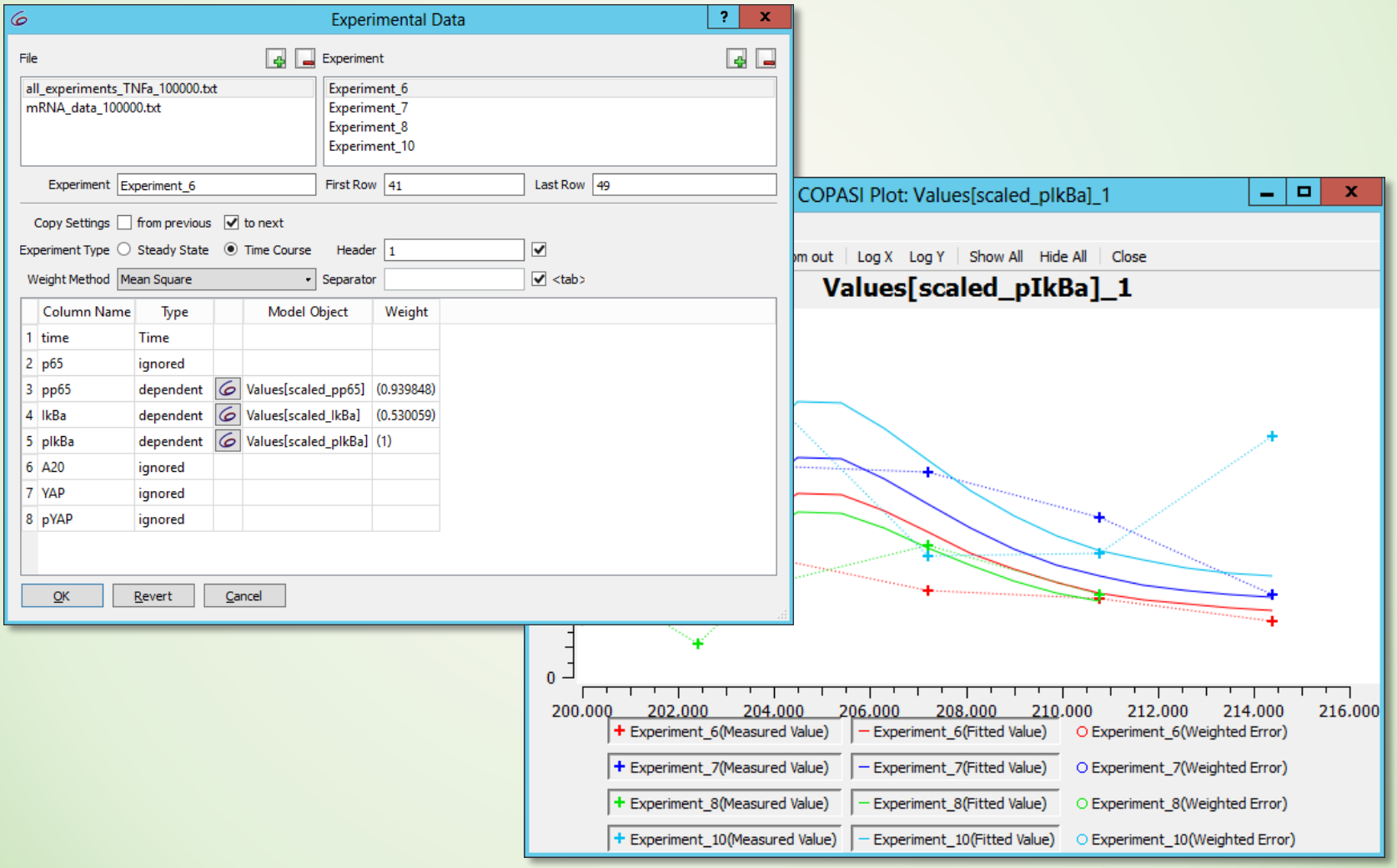
Python Simulator for Cellular Systems

SED-ML Web Tools



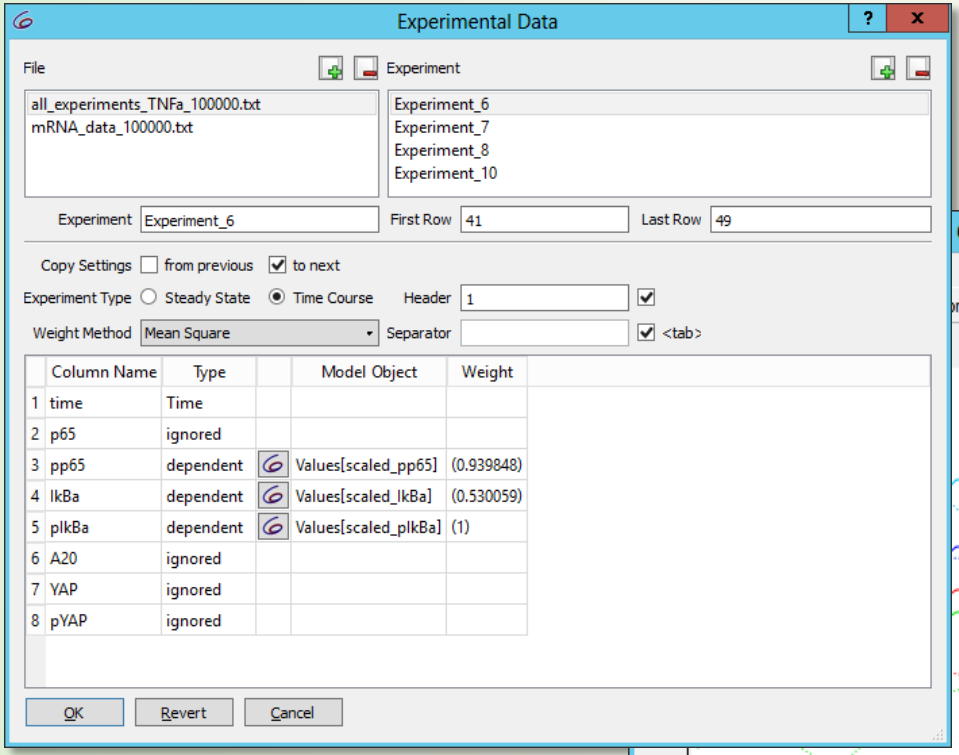
http://sysbioapps.dyndns.org/SED-ML_Web_Tools

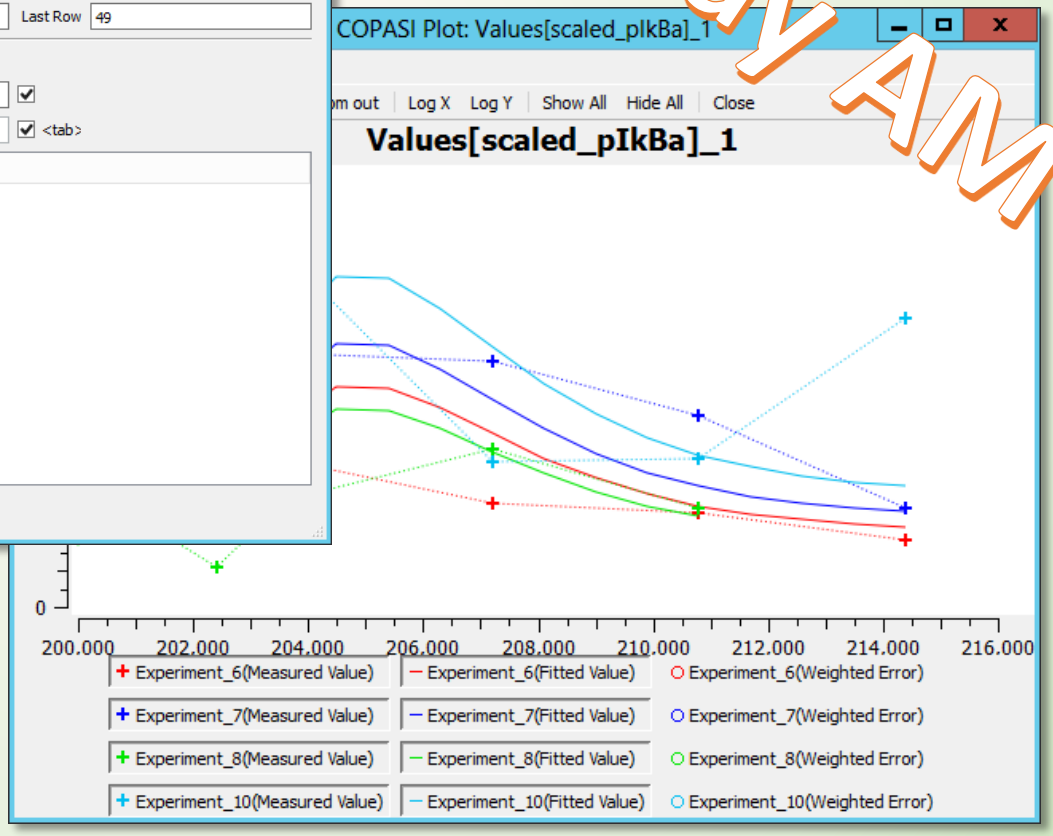
SED-ML Future



SED-ML Future

Wednesday AM





Acknowledgements

- SED-ML Editors: Frank T. Bergmann, Dagmar Waltemath, Jonathan Cooper, David Nickerson, Nicolas Le Novère, Andrew Miller, Richard Adams

- BioModels Support Team

- SED-ML Community