SBML Model Report

Model name: "Wang2009 - PI3K Ras Crosstalk"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Jason M Haugh[2] at January 21st 2010 at 1:25 p. m. and last time modified at February 14th 2014 at 11:33 a. m. Table 1 shows an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	19
events	0	constraints	0
reactions	13	function definitions	0
global parameters	45	unit definitions	0
rules	6	initial assignments	0

Model Notes

This model is from the article:
PI3K-dependent cross-talk interactions converge with Ras as quantifiable inputs integrated by Erk.

[1]EMBL-EBI, viji@ebi.ac.uk
[2]Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC, USA, jason_haugh@ncsu.edu

Wang CC, Cirit M, Haugh JM Mol. Syst. Biol. 2009;5:246. 19225459 ,

Abstract:
Although it is appreciated that canonical signal-transduction pathways represent dominant modes of regulation embedded in larger interaction networks, relatively little has been done to quantify pathway cross-talk in such networks. Through quantitative measurements that systematically canvas an array of stimulation and molecular perturbation conditions, together with computational modeling and analysis, we have elucidated cross-talk mechanisms in the platelet-derived growth factor (PDGF) receptor signaling network, in which phosphoinositide 3-kinase (PI3K) and Ras/extracellular signal-regulated kinase (Erk) pathways are prominently activated. We show that, while PI3K signaling is insulated from cross-talk, PI3K enhances Erk activation at points both upstream and downstream of Ras. The magnitudes of these effects depend strongly on the stimulation conditions, subject to saturation effects in the respective pathways and negative feedback loops. Motivated by those dynamics, a kinetic model of the network was formulated and used to precisely quantify the relative contributions of PI3K-dependent and -independent modes of Ras/Erk activation.

This model is parameterized with the median of the estimated parameters given in the supplementary material of the original publication's (doi: 10.1038/msb.2009.4) supplement on pages 8 and 9.

2 Unit Definitions

This is an overview of five unit definitions which are all predefined by SBML and not mentioned in the model.

2.1 Unit `substance`

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

2.2 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.3 Unit area

Notes Square metre is the predefined SBML unit for area since SBML Level 2 Version 1.

Definition m^2

2.4 Unit length

Notes Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

Definition m

2.5 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cell		0000290	3	1	litre	☑	

3.1 Compartment cell

This is a three dimensional compartment with a constant size of one litre.

SBO:0000290 physical compartment

4 Species

This model contains 19 species. Section 8 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
sumrc1		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
r		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
c1		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
c2		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ePI3K		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
m3PI		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
eGEF		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
mRas		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
x1		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
x2		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
y		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
yp		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ypp		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
z		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
zp		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
zpp		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
fGEF		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
w		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
eph		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 45 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
L		0000188	1.000		☑
KDL		0000282	1.500		☑
kxR0		0000009	0.300		☑
kminusx		0000009	0.007		☑
ke		0000009	0.200		☑
kt		0000009	0.005		☑
alphaPI3K		0000002	80.000		☑
kappaPI3K		0000282	0.300		☑
k3PI		0000002	1.000		☑
KGR		0000337	495.000		☑
KGP		0000337	5.090		☑
kRas		0000009	1.000		☑
Gamma		0000002	0.100		☑
kdx1		0000009	0.745		☑
kdx2		0000009	2.850		☑
Kx2		0000002	6.770		☑
VmaxOVERKMx11		0000002	1.180		☑
KMx11		0000027	30.300		☑
VmaxOVERKMx21		0000002	0.405		☑
KMx21		0000027	13.700		☑
VmaxOVERKMyph1		0000002	1.650		☑
KMyph1		0000027	23.000		☑
VmaxOVERKMx12		0000002	3.450		☑
KMx12		0000027	18.600		☑
VmaxOVERKMx22		0000002	1.090		☑
KMx22		0000027	9.590		☑
VmaxOVERKMyph2		0000002	4.200		☑
KMyph2		0000027	7.990		☑
VmaxOVERKMy1		0000002	6.570		☑
KMy1		0000027	9.910		☑
VmaxOVERKMzph1		0000002	0.167		☑
KMzph1		0000027	8.270		☑
VmaxOVERKMy2		0000002	31.900		☑
KMy2		0000027	8.810		☑
VmaxOVERKMzph2		0000002	0.228		☑
KMzph2		0000027	31.500		☑
kFBf		0000002	0.976		☑

Id	Name	SBO	Value	Unit	Constant
Zf		0000002	0.272		☑
n		0000190	1.030		☑
Kf		0000009	3.760		☑
kdw		0000009	0.033		☑
kFBph		0000009	2.340		☑
Wph		0000009	0.385		☑
p		0000190	1.980		☑
Kph		0000009	4.640		☑

6 Rules

This is an overview of six rules.

6.1 Rule r

Rule r is an assignment rule for species r:

$$\mathrm{r} = \frac{\mathrm{KDL} \cdot [\mathrm{sumrc1}]}{\mathrm{KDL} + \mathrm{L}} \tag{1}$$

6.2 Rule c1

Rule c1 is an assignment rule for species c1:

$$\mathrm{c1} = \frac{\mathrm{L} \cdot [\mathrm{sumrc1}]}{\mathrm{KDL} + \mathrm{L}} \tag{2}$$

6.3 Rule ePI3K

Rule ePI3K is an assignment rule for species ePI3K:

$$\mathrm{ePI3K} \tag{3}$$
$$= \frac{1 + \mathrm{kappaPI3K} + 2 \cdot \mathrm{alphaPI3K} \cdot [\mathrm{c2}] - \left((1 + \mathrm{kappaPI3K} + 2 \cdot \mathrm{alphaPI3K} \cdot [\mathrm{c2}])^2 - 8 \cdot \mathrm{alphaPI3K} \cdot [\mathrm{c2}] \right)^{0.5}}{2}$$

6.4 Rule eGEF

Rule eGEF is an assignment rule for species eGEF:

$$\mathrm{eGEF} = \frac{\mathrm{KGR} \cdot [\mathrm{c2}] + \mathrm{KGP} \cdot [\mathrm{m3PI}]}{1 + \mathrm{KGR} \cdot [\mathrm{c2}] + \mathrm{KGP} \cdot [\mathrm{m3PI}]} \cdot [\mathrm{fGEF}] \tag{4}$$

6.5 Rule yp

Rule yp is an assignment rule for species yp:

$$\mathrm{yp} = 1 - [\mathrm{y}] - [\mathrm{ypp}] \tag{5}$$

6.6 Rule zp

Rule zp is an assignment rule for species zp:

$$\mathrm{zp} = 1 - [\mathrm{z}] - [\mathrm{zpp}] \tag{6}$$

7 Reactions

This model contains 13 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	sumrc1ODE		$\emptyset \xrightleftharpoons{c2,\ c1} sumrc1$	
2	c2ODE		$\emptyset \xrightleftharpoons{c1} c2$	
3	m3PIODE		$\emptyset \xrightleftharpoons{ePI3K} m3PI$	
4	mRasODE		$\emptyset \xrightleftharpoons{eGEF} mRas$	
5	x1ODE		$\emptyset \xrightleftharpoons{mRas,\ y,\ yp} x1$	
6	x2ODE		$\emptyset \xrightleftharpoons{m3PI,\ y,\ yp} x2$	
7	yODE		$\emptyset \xrightleftharpoons{yp,\ ypp,\ x1,\ x2} y$	
8	yppODE		$\emptyset \xrightleftharpoons{x1,\ yp,\ y,\ x2,\ z,\ zp} ypp$	
9	zODE		$\emptyset \xrightleftharpoons{eph,\ zp,\ zpp,\ ypp} z$	
10	zppODE		$\emptyset \xrightleftharpoons{ypp,\ zp,\ z,\ eph} zpp$	
11	fGEFODE		$\emptyset \xrightleftharpoons{zpp} fGEF$	
12	wODE		$\emptyset \xrightleftharpoons{zpp} w$	
13	ephODE		$\emptyset \xrightleftharpoons{w} eph$	

7.1 Reaction `sumrc1ODE`

This is a reversible reaction of no reactant forming one product influenced by two modifiers.

Reaction equation

$$\emptyset \overset{\text{c2, c1}}{\rightleftharpoons} \text{sumrc1} \tag{7}$$

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
c2		
c1		

Product

Table 7: Properties of each product.

Id	Name	SBO
sumrc1		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{kt} \cdot (1 - [\text{sumrc1}]) + 2 \cdot \left(\text{kminusx} \cdot [\text{c2}] - \text{kxR0} \cdot [\text{c1}]^2\right) \tag{8}$$

7.2 Reaction `c2ODE`

This is a reversible reaction of no reactant forming one product influenced by one modifier.

Reaction equation

$$\emptyset \overset{\text{c1}}{\rightleftharpoons} \text{c2} \tag{9}$$

Modifier

Table 8: Properties of each modifier.

Id	Name	SBO
c1		

Product

Table 9: Properties of each product.

Id	Name	SBO
c2		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{kxR0} \cdot [\mathrm{c1}]^2 - (\mathrm{kminusx} + \mathrm{ke}) \cdot [\mathrm{c2}] \tag{10}$$

7.3 Reaction m3PIODE

This is a reversible reaction of no reactant forming one product influenced by one modifier.

Reaction equation

$$\emptyset \xrightleftharpoons{\mathrm{ePI3K}} \mathrm{m3PI} \tag{11}$$

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
ePI3K		

Product

Table 11: Properties of each product.

Id	Name	SBO
m3PI		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{k3PI} \cdot ([\text{ePI3K}] - [\text{m3PI}]) \tag{12}$$

7.4 Reaction mRasODE

This is a reversible reaction of no reactant forming one product influenced by one modifier.

Reaction equation

$$\emptyset \xrightleftharpoons{\text{eGEF}} \text{mRas} \tag{13}$$

Modifier

Table 12: Properties of each modifier.

Id	Name	SBO
eGEF		

Product

Table 13: Properties of each product.

Id	Name	SBO
mRas		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{kRas} \cdot ((1 + \text{Gamma}) \cdot [\text{eGEF}] - (1 + \text{Gamma} \cdot [\text{eGEF}]) \cdot [\text{mRas}]) \tag{14}$$

7.5 Reaction x1ODE

This is a reversible reaction of no reactant forming one product influenced by three modifiers.

Reaction equation

$$\emptyset \xrightleftharpoons{\text{mRas, y, yp}} \text{x1} \tag{15}$$

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
mRas		
y		
yp		

Product

Table 15: Properties of each product.

Id	Name	SBO
x1		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{kdx1} \cdot \left([\mathrm{mRas}] - \frac{[\mathrm{x1}]}{1 + \frac{[\mathrm{y}]}{\mathrm{KMx11}} + \frac{[\mathrm{yp}]}{\mathrm{KMx12}}} \right) \tag{16}$$

7.6 Reaction x20DE

This is a reversible reaction of no reactant forming one product influenced by three modifiers.

Reaction equation

$$\emptyset \xrightleftharpoons{\mathrm{m3PI,\ y,\ yp}} \mathrm{x2} \tag{17}$$

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
m3PI		
y		
yp		

Product

Table 17: Properties of each product.

Id	Name	SBO
x2		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{kdx2} \cdot \left(\frac{(1 + \text{Kx2}) \cdot [\text{m3PI}]}{1 + \text{Kx2} \cdot [\text{m3PI}]} - \frac{[\text{x2}]}{1 + \frac{[\text{y}]}{\text{KMx21}} + \frac{[\text{yp}]}{\text{KMx22}}} \right) \tag{18}$$

7.7 Reaction yODE

This is a reversible reaction of no reactant forming one product influenced by four modifiers.

Reaction equation

$$\emptyset \xrightleftharpoons{\text{yp, ypp, x1, x2}} \text{y} \tag{19}$$

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
yp		
ypp		
x1		
x2		

Product

Table 19: Properties of each product.

Id	Name	SBO
y		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\mathrm{VmaxOVERKMyph1} \cdot [\mathrm{yp}]}{1 + \frac{[\mathrm{yp}]}{\mathrm{KMyph1}} + \frac{[\mathrm{ypp}]}{\mathrm{KMyph2}}} - \frac{\mathrm{VmaxOVERKMx11} \cdot [\mathrm{x1}] \cdot [\mathrm{y}]}{1 + \frac{[\mathrm{y}]}{\mathrm{KMx11}} + \frac{[\mathrm{yp}]}{\mathrm{KMx12}}} - \frac{\mathrm{VmaxOVERKMx21} \cdot [\mathrm{x2}] \cdot [\mathrm{y}]}{1 + \frac{[\mathrm{y}]}{\mathrm{KMx21}} + \frac{[\mathrm{yp}]}{\mathrm{KMx22}}} \tag{20}$$

7.8 Reaction yppODE

This is a reversible reaction of no reactant forming one product influenced by six modifiers.

Reaction equation

$$\emptyset \xrightleftharpoons{\mathrm{x1,\ yp,\ y,\ x2,\ z,\ zp}} \mathrm{ypp} \tag{21}$$

Modifiers

Table 20: Properties of each modifier.

Id	Name	SBO
x1		
yp		
y		
x2		
z		
zp		

Product

Table 21: Properties of each product.

Id	Name	SBO
ypp		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\mathrm{VmaxOVERKMx12} \cdot [\mathrm{x1}] \cdot [\mathrm{yp}]}{1 + \frac{[\mathrm{y}]}{\mathrm{KMx11}} + \frac{[\mathrm{yp}]}{\mathrm{KMx12}}} + \frac{\mathrm{VmaxOVERKMx22} \cdot [\mathrm{x2}] \cdot [\mathrm{yp}]}{1 + \frac{[\mathrm{y}]}{\mathrm{KMx21}} + \frac{[\mathrm{yp}]}{\mathrm{KMx22}}} - \frac{\mathrm{VmaxOVERKMyph2} \cdot [\mathrm{ypp}]}{\left(1 + \frac{[\mathrm{z}]}{\mathrm{KMy1}} + \frac{[\mathrm{zp}]}{\mathrm{KMy2}}\right) \cdot \left(1 + \frac{[\mathrm{yp}]}{\mathrm{KMyph1}}\right) + \frac{[\mathrm{ypp}]}{\mathrm{KMyph2}}} \tag{22}$$

7.9 Reaction zODE

This is a reversible reaction of no reactant forming one product influenced by four modifiers.

Reaction equation

$$\emptyset \rightleftharpoons \mathrm{z} \quad \text{(eph, zp, zpp, ypp)} \tag{23}$$

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
eph		
zp		
zpp		
ypp		

Product

Table 23: Properties of each product.

Id	Name	SBO
z		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \frac{\mathrm{VmaxOVERKMzph1} \cdot [\mathrm{eph}] \cdot [\mathrm{zp}]}{1 + \frac{[\mathrm{zp}]}{\mathrm{KMzph1}} + \frac{[\mathrm{zpp}]}{\mathrm{KMzph2}}} - \frac{\mathrm{VmaxOVERKMy1} \cdot [\mathrm{ypp}] \cdot [\mathrm{z}]}{1 + \frac{[\mathrm{z}]}{\mathrm{KMy1}} + \frac{[\mathrm{zp}]}{\mathrm{KMy2}}} \tag{24}$$

7.10 Reaction zppODE

This is a reversible reaction of no reactant forming one product influenced by four modifiers.

Reaction equation

$$\emptyset \underset{}{\overset{\text{ypp, zp, z, eph}}{\rightleftharpoons}} \text{zpp} \tag{25}$$

Modifiers

Table 24: Properties of each modifier.

Id	Name	SBO
ypp		
zp		
z		
eph		

Product

Table 25: Properties of each product.

Id	Name	SBO
zpp		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \frac{\text{VmaxOVERKMy2} \cdot [\text{ypp}] \cdot [\text{zp}]}{1 + \frac{[\text{z}]}{\text{KMy1}} + \frac{[\text{zp}]}{\text{KMy2}}} - \frac{\text{VmaxOVERKMzph2} \cdot [\text{eph}] \cdot [\text{zpp}]}{1 + \frac{[\text{zp}]}{\text{KMzph1}} + \frac{[\text{zpp}]}{\text{KMzph2}}} \tag{26}$$

7.11 Reaction `fGEFODE`

This is a reversible reaction of no reactant forming one product influenced by one modifier.

Reaction equation

$$\emptyset \underset{}{\overset{\text{zpp}}{\rightleftharpoons}} \text{fGEF} \tag{27}$$

Modifier

Table 26: Properties of each modifier.

Id	Name	SBO
zpp		

Product

Table 27: Properties of each product.

Id	Name	SBO
fGEF		

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{kFBf} \cdot \left(\frac{1 - [\mathrm{fGEF}]}{\mathrm{Kf}} - \frac{[\mathrm{zpp}]^{\mathrm{n}}}{\mathrm{Zf}^{\mathrm{n}} + [\mathrm{zpp}]^{\mathrm{n}}} \cdot [\mathrm{fGEF}] \right) \tag{28}$$

7.12 Reaction wODE

This is a reversible reaction of no reactant forming one product influenced by one modifier.

Reaction equation

$$\emptyset \overset{\mathrm{zpp}}{\rightleftharpoons} \mathrm{w} \tag{29}$$

Modifier

Table 28: Properties of each modifier.

Id	Name	SBO
zpp		

Product

Table 29: Properties of each product.

Id	Name	SBO
w		

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{kdw} \cdot ([\mathrm{zpp}] - [\mathrm{w}]) \tag{30}$$

7.13 Reaction `ephODE`

This is a reversible reaction of no reactant forming one product influenced by one modifier.

Reaction equation

$$\emptyset \overset{\mathrm{w}}{\rightleftharpoons} \mathrm{eph} \tag{31}$$

Modifier

Table 30: Properties of each modifier.

Id	Name	SBO
`w`		

Product

Table 31: Properties of each product.

Id	Name	SBO
`eph`		

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{kFBph} \cdot \left(\frac{[\mathrm{w}]^{\mathrm{p}}}{\mathrm{Wph}^{\mathrm{p}} + [\mathrm{w}]^{\mathrm{p}}} - \frac{[\mathrm{eph}] - 1}{\mathrm{Kph}} \right) \tag{32}$$

8 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML `substance` per `time`. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or
- volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions`> 0 for certain species.

8.1 Species `sumrc1`

SBO:0000296 macromolecular complex

Initial concentration $1\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a product in `sumrc1ODE`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{sumrc1} = v_1 \tag{33}$$

8.2 Species `r`

SBO:0000245 macromolecule

Involved in rule `r`

One rule which determines this species' quantity.

8.3 Species `c1`

SBO:0000296 macromolecular complex

Involved in rule `c1`

This species takes part in two reactions (as a modifier in `sumrc1ODE`, `c2ODE`) and is also involved in one rule which determines this species' quantity.

8.4 Species `c2`

SBO:0000420 multimer of macromolecules

Initial concentration $0\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a product in `c2ODE` and as a modifier in `sumrc1ODE`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{c2} = v_2 \tag{34}$$

8.5 Species `ePI3K`

SBO:0000245 macromolecule

Involved in rule `ePI3K`

This species takes part in one reaction (as a modifier in `m3PIODE`) and is also involved in one rule which determines this species' quantity.

8.6 Species m3PI

SBO:0000236 physical entity representation

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a product in m3PIODE and as a modifier in x2ODE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{m3PI} = v_3 \tag{35}$$

8.7 Species eGEF

Involved in rule eGEF

This species takes part in one reaction (as a modifier in mRasODE) and is also involved in one rule which determines this species' quantity.

8.8 Species mRas

SBO:0000245 macromolecule

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a product in mRasODE and as a modifier in x1ODE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{mRas} = v_4 \tag{36}$$

8.9 Species x1

SBO:0000014 enzyme

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a product in x1ODE and as a modifier in yODE, yppODE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x1} = v_5 \tag{37}$$

8.10 Species x2

SBO:0000014 enzyme

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a product in x2ODE and as a modifier in yODE, yppODE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x2} = v_6 \tag{38}$$

8.11 Species y

SBO:0000245 macromolecule

Initial concentration $1\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a product in yODE and as a modifier in x1ODE, x2ODE, yppODE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y} = v_7 \tag{39}$$

8.12 Species yp

SBO:0000245 macromolecule

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

Involved in rule yp

This species takes part in four reactions (as a modifier in x1ODE, x2ODE, yODE, yppODE) and is also involved in one rule which determines this species' quantity.

8.13 Species ypp

SBO:0000245 macromolecule

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a product in yppODE and as a modifier in yODE, zODE, zppODE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ypp} = v_8 \tag{40}$$

8.14 Species z

SBO:0000245 macromolecule

Initial concentration $1\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a product in zODE and as a modifier in yppODE, zppODE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{z} = v_9 \tag{41}$$

8.15 Species zp

SBO:0000245 macromolecule

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

Involved in rule zp

This species takes part in three reactions (as a modifier in yppODE, zODE, zppODE) and is also involved in one rule which determines this species' quantity.

8.16 Species zpp

SBO:0000245 macromolecule

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a product in zppODE and as a modifier in zODE, fGEFODE, wODE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{zpp} = v_{10} \tag{42}$$

8.17 Species fGEF

SBO:0000245 macromolecule

Initial concentration $1\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a product in fGEFODE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{fGEF} = v_{11} \tag{43}$$

8.18 Species w

SBO:0000245 macromolecule

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a product in wODE and as a modifier in ephODE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{w} = v_{12} \tag{44}$$

8.19 Species eph

SBO:0000245 macromolecule

Initial concentration $1\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a product in ephODE and as a modifier in zODE, zppODE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{eph} = v_{13} \tag{45}$$

A Glossary of Systems Biology Ontology Terms

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

SBO:0000009 kinetic constant: Numerical parameter that quantifies the velocity of a chemical reaction

SBO:0000014 enzyme: A protein that catalyzes a chemical reaction. The word comes from en “a” or“i”) and simo “leave” or“yeas”)

SBO:0000027 Michaelis constant: Substrate concentration at which the velocity of reaction is half its maximum. Michaelis constant is an experimental parameter. According to the underlying molecular mechanism it can be interpreted differently in terms of microscopic constants

SBO:0000188 number of biochemical items: A number of objects of the same type, identical or different, involved in a biochemical event

SBO:0000190 Hill coefficient: Empirical parameter created by Archibald Vivian Hill to describe the cooperative binding of oxygen on hemoglobine (Hill (1910). The possible effects of the aggregation of the molecules of haemoglobin on its dissociation curves. J Physiol 40: iv-vii)

SBO:0000236 physical entity representation: Representation of an entity that may participate in an interaction, a process or relationship of significance.

SBO:0000245 macromolecule: Molecular entity mainly built-up by the repetition of pseudo-identical units. CHEBI:3383

SBO:0000282 dissociation constant: Equilibrium constant that measures the propensity of a larger object to separate (dissociate) reversibly into smaller components, as when a complex falls apart into its component molecules, or when a salt splits up into its component ions. The dissociation constant is usually denoted Kd and is the inverse of the affinity constant.

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

SBO:0000296 macromolecular complex: Non-covalent complex of one or more macromolecules and zero or more simple chemicals

SBO:0000337 association constant: Equilibrium constant that measures the propensity of two objects to assemble (associate) reversibly into a larger component. The association constant is usually denoted Ka and is the inverse of the dissociation constant.

SBO:0000420 multimer of macromolecules: Non-covalent association between several macromolecule

SBML2LaTeX was developed by Andreas Dräger[a], Hannes Planatscher[a], Dieudonné M Wouamba[a], Adrian Schröder[a], Michael Hucka[b], Lukas Endler[c], Martin Golebiewski[d] and Andreas Zell[a]. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany