SBML Model Report

Model name: "Schaber2006_Pheromone-Starvation_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 three authors: Lukas Endler¹, Vijayalakshmi Chelliah² and Jorg Schaber³ at August 20th 2009 at 5:18 p. m. and last time modified at April eighth 2016 at 4:03 p. m. Table 1 provides 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	26
events	0	constraints	0
reactions	31	function definitions	0
global parameters	46	unit definitions	0
rules	2	initial assignments	0

Model Notes

This a model from the article:

A modelling approach to quantify dynamic crosstalk between the pheromone and the starvation pathway in baker's yeast.

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Schaber J, Kofahl B, Kowald A, Klipp E <u>FEBS J.</u>2006 Aug; 273(15):3520-33 16884493, **Abstract:**

Cells must be able to process multiple information in parallel and, moreover, they must also be able to combine this information in order to trigger the appropriate response. This is achieved by wiring signalling pathways such that they can interact with each other, a phenomenon often called crosstalk. In this study, we employ mathematical modelling techniques to analyse dynamic mechanisms and measures of crosstalk. We present a dynamic mathematical model that compiles current knowledge about the wiring of the pheromone pathway and the filamentous growth pathway in yeast. We consider the main dynamic features and the interconnections between the two pathways in order to study dynamic crosstalk between these two pathways in haploid cells. We introduce two new measures of dynamic crosstalk, the intrinsic specificity and the extrinsic specificity. These two measures incorporate the combined signal of several stimuli being present simultaneously and seem to be more stable than previous measures. When both pathways are responsive and stimulated, the model predicts that (a) the filamentous growth pathway amplifies the response of the pheromone pathway, and (b) the pheromone pathway inhibits the response of filamentous growth pathway in terms of mitogen activated protein kinase activity and transcriptional activity, respectively. Among several mechanisms we identified leakage of activated Stell as the most influential source of crosstalk. Moreover, we propose new experiments and predict their outcomes in order to test hypotheses about the mechanisms of crosstalk between the two pathways. Studying signals that are transmitted in parallel gives us new insights about how pathways and signals interact in a dynamical way, e.g., whether they amplify, inhibit, delay or accelerate each other.

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To cite BioModels Database, please use Le Novre N., Bornstein B., Broicher A., Courtot M., Donizelli M., Dharuri H., Li L., Sauro H., Schilstra M., Shapiro B., Snoep J.L., Hucka M. (2006) BioModels Database: A Free, Centralized Database of Curated, Published, Quantitative Kinetic Models of Biochemical and Cellular Systems Nucleic Acids Res., 34: D689-D691.

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 1

2.3 Unit area

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

Definition m²

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
compartment	compartment	0000290	3	1	litre	Ø	

3.1 Compartment compartment

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

Name compartment

SBO:0000290 physical compartment

4 Species

This model contains 26 species. The boundary condition of two of these species is set to true so that these species' amount cannot be changed by any reaction. 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 Condi- tion
 Ste5	Ste5	compartment	$\text{mol} \cdot l^{-1}$		
Ste11	Ste11	compartment	$\text{mol} \cdot 1^{-1}$		
Ste5Ste11	Ste5Ste11	compartment	$\text{mol} \cdot 1^{-1}$		
Gbg	Gbg	compartment	$\text{mol} \cdot l^{-1}$		
Ste5Ste11Gbg	Ste5Ste11Gbg	compartment	$\text{mol} \cdot l^{-1}$		
Fus3	Fus3	compartment	$\text{mol} \cdot l^{-1}$		
Ste5Ste11GbgFus3	Ste5Ste11GbgFus3	compartment	$\text{mol} \cdot l^{-1}$		
Ste5Ste11GbgFus3P	Ste5Ste11GbgFus3P	compartment	$\mathrm{mol}\cdot \mathrm{l}^{-1}$		
Fus3PP	Fus3PP	compartment	$\text{mol} \cdot l^{-1}$		\Box
Ste5Ste11GbgP	Ste5Ste11GbgP	compartment	$\text{mol} \cdot l^{-1}$		\Box
Ste11Ubi	Ste11Ubi	compartment	$\text{mol} \cdot l^{-1}$		\Box
p	p	compartment	$\text{mol} \cdot l^{-1}$		\square
Kss1	Kss1	compartment	$\text{mol} \cdot l^{-1}$		
Ste5Ste11GbgKss1	Ste5Ste11GbgKss1	compartment	$\text{mol} \cdot l^{-1}$		\Box
Ste5Ste11GbgKss1P	Ste5Ste11GbgKss1P	compartment	$\text{mol} \cdot l^{-1}$		\Box
Kss1PP	Kss1PP	compartment	$\text{mol} \cdot l^{-1}$		\Box
Ste11P	Ste11P	compartment	$\text{mol} \cdot l^{-1}$		
Ste12Kss1	Ste12Kss1	compartment	$\text{mol} \cdot l^{-1}$		
Ste12	Ste12	compartment	$\text{mol} \cdot l^{-1}$		
Ste12P	Ste12P	compartment	$\operatorname{mol} \cdot 1^{-1}$		\Box
s	S	compartment	$\text{mol} \cdot l^{-1}$		

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
PREP	PREP	compartment	$\text{mol} \cdot l^{-1}$		
Ste12TeSte5Kss1	Ste12TeSte5Kss1	compartment	$\text{mol} \cdot 1^{-1}$		
Ste12TeSte5	Ste12TeSte5	compartment	$\text{mol} \cdot l^{-1}$		
Ste12TeSte5P	Ste12TeSte5P	compartment	$\text{mol} \cdot l^{-1}$		
FREP	FREP	${\tt compartment}$	$\text{mol} \cdot l^{-1}$		

5 Parameters

This model contains 46 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO Value	Unit	Constant
alpha		0.00		
beta		0.00		
alphaA	alphaA	1.00		
betaA	betaA	1.00		
alphat	alphat	0.00		
betat	betat	0.00		
alphas	alphas	2.00		
betas	betas	20.00		$ \overline{\mathbf{Z}} $
alphae	alphae	10.00		
betae	betae	360.00		
k3	k3	1.00		$ \overline{\checkmark} $
k4	k4	1.00		
k5	k5	1.00		
k6	k6	1.00		$ \overline{\mathbf{Z}} $
k9	k9	1.00		$ \overline{\mathbf{Z}} $
k10	k10	1.00		$ \overline{\mathbf{Z}} $
k11	k11	1.00		$ \overline{\mathbf{Z}} $
k12	k12	1.00		
k13	k13	1.00		
k17	k17	1.00		
k19	k19	1.00		$ \overline{\mathbf{Z}} $
k20	k20	1.00		
k21	k21	1.00		
k22	k22	1.00		
k23	k23	1.00		
k25	k25	1.00		
k27	k27	1.00		
k31	k31	1.00		$ \overline{\checkmark} $
k32	k32	1.00		$ \overline{\mathbf{Z}} $
k33	k33	1.00		
k34	k34	1.00		$\overline{\mathbf{Z}}$
k8	k8	0.10		$\overline{\mathbf{Z}}$
k14	k14	0.10		$\overline{\mathbf{Z}}$
k15	k15	0.10		$\overline{\mathbf{Z}}$
k16	k16	0.10		$\overline{\mathbb{Z}}$
k26	k26	0.10		$\overline{\mathbb{Z}}$
k30	k30	0.10		$\overline{\mathbf{Z}}$

Id	Name	SBO Value	Unit	Constant
k7	k7	10.00)	\overline{Z}
k18	k18	10.00)	$\overline{\mathbf{Z}}$
k1	k1	0.01		
k2	k2	0.01		
k24	k24	0.01		
k28	k28	0.01		
k29	k29	0.01		
alphastim	alphastim	1.00)	
betastim	betastim	1.00)	\square

6 Rules

This is an overview of two rules.

6.1 Rule alpha

Rule alpha is an assignment rule for parameter alpha:

6.2 Rule beta

Rule beta is an assignment rule for parameter beta:

$$beta = betastim \cdot betaA$$

$$\begin{cases}
1 - exp\left(\frac{(time - betat)}{betas}\right) & \text{if } (time \ge betat) \land (time \le betae) \\
\begin{cases}
exp\left(\frac{(time - betae)}{betas}\right) & \text{if } time > betae \\
0 & \text{otherwise}
\end{cases}$$
otherwise

Produced by SBML2PTEX

7 Reactions

This model contains 31 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

N⁰	Id	Name	Reaction Equation	SBO
1	v1	v1	Ste5+Ste11 ⇒ Ste5Ste11	0000177
2	v2	v2	$Ste5Ste11 + Gbg \Longrightarrow Ste5Ste11Gbg$	0000177
3	v3	v3	$Ste5Ste11Gbg + Fus3 \Longrightarrow Ste5Ste11GbgFus3$	0000177
4	v4	v4	$Ste5Ste11GbgFus3 \Longrightarrow Ste5Ste11GbgFus3P$	0000216
5	v5	v5	$Ste5Ste11GbgFus3P \Longrightarrow Fus3PP +$	0000216
			Ste5Ste11GbgP	
6	v6	v6	$Fus3 + Ste5Ste11GbgP \Longrightarrow Ste5Ste11GbgFus3P$	0000177
7	v7	v7	$Ste5 + Ste5Ste11GbgP \Longrightarrow Gbg + Ste11Ubi$	0000180
8	v8	v8	Ste11Ubi ← p	0000179
9	v9	v9	$Ste5Ste11Gbg + Kss1 \Longrightarrow Ste5Ste11GbgKss1$	0000177
10	v10	v10	Ste5Ste11GbgKss1 ← Ste5Ste11GbgKss1P	0000216
11	v11	v11	$Ste5Ste11GbgKss1P \Longrightarrow Ste5Ste11GbgP +$	0000216
			Kss1PP	
12	v12	v12	$Ste5Ste11GbgP + Kss1 \Longrightarrow Ste5Ste11GbgKss1P$	0000177
13	v13	v13	$Ste11 \Longrightarrow Ste11P$	0000216
14	v14	v14	$Ste11P \Longrightarrow Ste11$	0000330
15	1 E	w15	$Kss1 \xrightarrow{Ste11P, Ste11Ubi} Kss1PP$	0000216
13	v15	v15		0000210
16	v16	v16	$Kss1PP \xrightarrow{Fus3PP} Kss1$	0000330
17	v17	v17	$Ste12Kss1 \Longrightarrow 2Kss1 + Ste12$	0000180
18	v18	v18	$2 \text{ Kss} 1 + \text{Ste} 12 \Longrightarrow \text{Ste} 12 \text{Kss} 1$	0000177
19	v19	v19	Ste12 Fus3PP, Kss1PP Ste12P	0000216

N⁰	Id	Name	Reaction Equation	SBO
20	v20	v20	$s \stackrel{\text{Ste12P}}{=\!=\!=\!=} PREP$	0000205
21	v21	v21	$Ste12TeSte5Kss1 \Longrightarrow Kss1 + Ste12TeSte5$	0000180
22	v22	v22	$Kss1 + Ste12TeSte5 \Longrightarrow Ste12TeSte5Kss1$	0000177
23	v23	v23	Ste12TeSte5 $\stackrel{Kss1PP}{\longleftarrow}$ Ste12TeSte5P	0000216
24	v24	v24	Ste12TeSte5 $\stackrel{\text{Fus3PP}}{\longleftarrow}$ p	0000179
25	v25	v25	s Ste12TeSte5P FREP	0000205
26	v26	v26	Fus3PP ← Fus3	0000330
27	v27	v27	$Ste5Ste11 \Longrightarrow Ste5 + Ste11$	0000180
28	v28	v28	$Ste12P \Longrightarrow Ste12$	0000330
29	v29	v29	$PREP \rightleftharpoons p$	0000179
30	v30	v30	Ste12TeSte5P	0000330
31	v31	v31	$FREP \rightleftharpoons p$	0000179

7.1 Reaction v1

This is a reversible reaction of two reactants forming one product.

Name v1

SBO:0000177 non-covalent binding

Reaction equation

$$Ste5 + Ste11 \Longrightarrow Ste5Ste11$$
 (3)

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
Ste5	Ste5	
Ste11	Ste11	

Product

Table 7: Properties of each product.

Id	Name	SBO
Ste5Ste11	Ste5Ste11	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\left(\text{compartment}\right) \cdot \text{k1} \cdot [\text{Ste5}] \cdot [\text{Ste11}]$$
 (4)

7.2 Reaction v2

This is a reversible reaction of two reactants forming one product.

Name v2

SBO:0000177 non-covalent binding

Reaction equation

$$Ste5Ste11 + Gbg \Longrightarrow Ste5Ste11Gbg$$
 (5)

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
Ste5Ste11	Ste5Ste11	
Gbg	Gbg	

Product

Table 9: Properties of each product.

Id	Name	SBO
Ste5Ste11Gbg	Ste5Ste11Gbg	-

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol} (\text{compartment}) \cdot \text{k2} \cdot [\text{Ste5Ste11}] \cdot [\text{Gbg}] \cdot \text{alpha}$$
 (6)

7.3 Reaction v3

This is a reversible reaction of two reactants forming one product.

Name v3

SBO:0000177 non-covalent binding

Reaction equation

$$Ste5Ste11Gbg + Fus3 \Longrightarrow Ste5Ste11GbgFus3 \tag{7}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
Ste5Ste11Gbg Fus3	Ste5Ste11Gbg Fus3	

Product

Table 11: Properties of each product.

Id	Name	SBO
Ste5Ste11GbgFus3	Ste5Ste11GbgFus3	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{compartment}) \cdot \text{k3} \cdot [\text{Ste5Ste11Gbg}] \cdot [\text{Fus3}]$$
 (8)

7.4 Reaction v4

This is a reversible reaction of one reactant forming one product.

Name v4

SBO:0000216 phosphorylation

Reaction equation

$$Ste5Ste11GbgFus3 \Longrightarrow Ste5Ste11GbgFus3P \tag{9}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Ste5Ste11GbgFus3	Ste5Ste11GbgFus3	

Product

Table 13: Properties of each product.

Id	Name	SBO
Ste5Ste11GbgFus3P	Ste5Ste11GbgFus3P	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol} (\text{compartment}) \cdot \text{k4} \cdot [\text{Ste5Ste11GbgFus3}]$$
 (10)

7.5 Reaction v5

This is a reversible reaction of one reactant forming two products.

Name v5

SBO:0000216 phosphorylation

Reaction equation

$$Ste5Ste11GbgFus3P \Longrightarrow Fus3PP + Ste5Ste11GbgP$$
 (11)

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
Ste5Ste11GbgFus3P	Ste5Ste11GbgFus3P	

Products

Table 15: Properties of each product.

Id	Name	SBO
Fus3PP	Fus3PP	
Ste5Ste11GbgP	Ste5Ste11GbgP	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol} (\text{compartment}) \cdot \text{k5} \cdot [\text{Ste5Ste11GbgFus3P}]$$
 (12)

7.6 Reaction v6

This is a reversible reaction of two reactants forming one product.

Name v6

SBO:0000177 non-covalent binding

Reaction equation

$$Fus3 + Ste5Ste11GbgP \Longrightarrow Ste5Ste11GbgFus3P$$
 (13)

Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
Fus3 Ste5Ste11GbgP	Fus3 Ste5Ste11GbgP	

Product

Table 17: Properties of each product.

Id	Name	SBO
Ste5Ste11GbgFus3P	Ste5Ste11GbgFus3P	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol} (\text{compartment}) \cdot \text{k6} \cdot [\text{Fus3}] \cdot [\text{Ste5Ste11GbgP}]$$
 (14)

7.7 Reaction v7

This is a reversible reaction of two reactants forming two products.

Name v7

SBO:0000180 dissociation

Reaction equation

$$Ste5 + Ste5Ste11GbgP \Longrightarrow Gbg + Ste11Ubi$$
 (15)

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
Ste5	Ste5	
Ste5Ste11GbgP	Ste5Ste11GbgP	

Products

Table 19: Properties of each product.

Id	Name	SBO
Gbg	Gbg	
Ste11Ubi	Ste11Ubi	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol} (\text{compartment}) \cdot \text{k7} \cdot [\text{Ste5Ste11GbgP}]$$
 (16)

7.8 Reaction v8

This is a reversible reaction of one reactant forming one product.

Name v8

SBO:0000179 degradation

Reaction equation

$$Ste11Ubi \rightleftharpoons p \tag{17}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
Ste11Ubi	Ste11Ubi	

Product

Table 21: Properties of each product.

Id	Name	SBO
р	p	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}\left(\text{compartment}\right) \cdot \text{k8} \cdot \left[\text{Ste11Ubi}\right]$$
 (18)

7.9 Reaction v9

This is a reversible reaction of two reactants forming one product.

Name v9

SBO:0000177 non-covalent binding

Reaction equation

$$Ste5Ste11Gbg + Kss1 \Longrightarrow Ste5Ste11GbgKss1$$
 (19)

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
Ste5Ste11Gbg Kss1	Ste5Ste11Gbg Kss1	

Product

Table 23: Properties of each product.

Id	Name	SBO
Ste5Ste11GbgKss1	Ste5Ste11GbgKss1	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol} (\text{compartment}) \cdot \text{k9} \cdot [\text{Ste5Ste11Gbg}] \cdot [\text{Kss1}]$$
 (20)

7.10 Reaction v10

This is a reversible reaction of one reactant forming one product.

Name v10

SBO:0000216 phosphorylation

Reaction equation

$$Ste5Ste11GbgKss1 \Longrightarrow Ste5Ste11GbgKss1P$$
 (21)

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
Ste5Ste11GbgKss1	Ste5Ste11GbgKss1	

Product

Table 25: Properties of each product.

Id	Name	SBO
Ste5Ste11GbgKss1P	Ste5Ste11GbgKss1P	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol} (\text{compartment}) \cdot \text{k}10 \cdot [\text{Ste5Ste11GbgKss1}]$$
 (22)

7.11 Reaction v11

This is a reversible reaction of one reactant forming two products.

Name v11

SBO:0000216 phosphorylation

Reaction equation

$$Ste5Ste11GbgKss1P \Longrightarrow Ste5Ste11GbgP + Kss1PP$$
 (23)

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
Ste5Ste11GbgKss1P	Ste5Ste11GbgKss1P	

Products

Table 27: Properties of each product.

Id	Name	SBO
Ste5Ste11GbgP Kss1PP	Ste5Ste11GbgP Kss1PP	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{vol}\left(\text{compartment}\right) \cdot \text{k11} \cdot \left[\text{Ste5Ste11GbgKss1P}\right]$$
 (24)

7.12 Reaction v12

This is a reversible reaction of two reactants forming one product.

Name v12

SBO:0000177 non-covalent binding

Reaction equation

$$Ste5Ste11GbgP + Kss1 \Longrightarrow Ste5Ste11GbgKss1P$$
 (25)

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
Ste5Ste11GbgP Kss1	Ste5Ste11GbgP Kss1	

Product

Table 29: Properties of each product.

Id	Name	SBO
Ste5Ste11GbgKss1P	Ste5Ste11GbgKss1P	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{vol}(\text{compartment}) \cdot \text{k12} \cdot [\text{Ste5Ste11GbgP}] \cdot [\text{Kss1}]$$
 (26)

7.13 Reaction v13

This is a reversible reaction of one reactant forming one product.

Name v13

SBO:0000216 phosphorylation

Reaction equation

$$Ste11 \Longrightarrow Ste11P \tag{27}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
Ste11	Ste11	

Product

Table 31: Properties of each product.

Id	Name	SBO
Ste11P	Ste11P	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{vol} (\text{compartment}) \cdot \text{k13} \cdot [\text{Ste11}] \cdot \text{beta}$$
 (28)

7.14 Reaction v14

This is a reversible reaction of one reactant forming one product.

Name v14

SBO:0000330 dephosphorylation

Reaction equation

$$Ste11P \Longrightarrow Ste11 \tag{29}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
Ste11P	Ste11P	

Product

Table 33: Properties of each product.

Id	Name	SBO
Ste11	Ste11	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol} \left(\text{compartment} \right) \cdot \text{k14} \cdot \left[\text{Ste11P} \right]$$
 (30)

7.15 Reaction v15

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name v15

SBO:0000216 phosphorylation

Reaction equation

$$Kss1 \xrightarrow{\underline{Ste11P, Ste11Ubi}} Kss1PP$$
 (31)

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
Kss1	Kss1	

Table 35: Properties of each modifier.

Id	Name	SBO
Ste11P	Ste11P	
Ste11Ubi	Ste11Ubi	

Table 36: Properties of each product.

Id	Name	SBO
Kss1PP	Kss1PP	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}\left(\text{compartment}\right) \cdot \left(\text{k15} \cdot \left[\text{Kss1}\right] \cdot \left[\text{Ste11P}\right] + \text{k30} \cdot \left[\text{Kss1}\right] \cdot \left[\text{Ste11Ubi}\right]\right)$$
 (32)

7.16 Reaction v16

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name v16

SBO:0000330 dephosphorylation

Reaction equation

$$Kss1PP \xrightarrow{Fus3PP} Kss1 \tag{33}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
Kss1PP	Kss1PP	

Table 38: Properties of each modifier.

Id	Name	SBO
Fus3PP	Fus3PP	

Table 39: Properties of each product.

Id	Name	SBO
Kss1	Kss1	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{vol} \left(\text{compartment} \right) \cdot \left(\text{k16} \cdot \left[\text{Kss1PP} \right] + \text{k28} \cdot \left[\text{Kss1PP} \right] \cdot \left[\text{Fus3PP} \right] \right)$$
 (34)

7.17 Reaction v17

This is a reversible reaction of one reactant forming two products.

Name v17

SBO:0000180 dissociation

Reaction equation

$$Ste12Kss1 \Longrightarrow 2Kss1 + Ste12 \tag{35}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
Ste12Kss1	Ste12Kss1	

Products

Table 41: Properties of each product.

Id	Name	SBO
Kss1	Kss1	
Ste12	Ste12	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{vol} \left(\text{compartment} \right) \cdot \text{k17} \cdot \left[\text{Ste12Kss1} \right]$$
 (36)

7.18 Reaction v18

This is a reversible reaction of two reactants forming one product.

Name v18

SBO:0000177 non-covalent binding

Reaction equation

$$2 \text{Kss1} + \text{Ste12} \Longrightarrow \text{Ste12Kss1}$$
 (37)

Reactants

Table 42: Properties of each reactant.

Id	Name	SBO
Kss1	Kss1	
Ste12	Ste12	

Product

Table 43: Properties of each product.

Id	Name	SBO
Ste12Kss1	Ste12Kss1	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol}(\text{compartment}) \cdot \text{k18} \cdot [\text{Kss1}] \cdot [\text{Ste12}]$$
 (38)

7.19 Reaction v19

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name v19

SBO:0000216 phosphorylation

Reaction equation

$$Ste12 \xrightarrow{Fus3PP, Kss1PP} Ste12P$$
 (39)

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
Ste12	Ste12	

Modifiers

Table 45: Properties of each modifier.

Id	Name	SBO
Fus3PP Kss1PP	Fus3PP Kss1PP	

Product

Table 46: Properties of each product.

Id	Name	SBO
Ste12P	Ste12P	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = vol(compartment) \cdot (k19 \cdot [Ste12] \cdot [Fus3PP] + k29 \cdot [Ste12] \cdot [Kss1PP])$$
 (40)

7.20 Reaction v20

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name v20

SBO:0000205 composite biochemical process

Reaction equation

$$s \stackrel{\underline{Ste12P}}{\longleftarrow} PREP \tag{41}$$

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
s	S	

Modifier

Table 48: Properties of each modifier.

Id	Name	SBO
Ste12P	Ste12P	

Product

Table 49: Properties of each product.

Id	Name	SBO
PREP	PREP	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}(\text{compartment}) \cdot \text{k20} \cdot [\text{Ste12P}]$$
 (42)

7.21 Reaction v21

This is a reversible reaction of one reactant forming two products.

Name v21

SBO:0000180 dissociation

Reaction equation

$$Ste12TeSte5Kss1 \Longrightarrow Kss1 + Ste12TeSte5$$
 (43)

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
Ste12TeSte5Kss1	Ste12TeSte5Kss1	

Products

Table 51: Properties of each product.

Id	Name	SBO
Kss1	Kss1	
Ste12TeSte5	Ste12TeSte5	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{vol}(\text{compartment}) \cdot \text{k21} \cdot [\text{Ste12TeSte5Kss1}]$$
 (44)

7.22 Reaction v22

This is a reversible reaction of two reactants forming one product.

Name v22

SBO:0000177 non-covalent binding

Reaction equation

$$Kss1 + Ste12TeSte5 \Longrightarrow Ste12TeSte5Kss1$$
 (45)

Reactants

Table 52: Properties of each reactant

Table 32. Properties of each feactain.		
Id	Name	SBO
Kss1 Ste12TeSte5	Kss1 Ste12TeSte5	
20012102000	21012103100	

Table 53: Properties of each product.

Id	Name	SBO
Ste12TeSte5Kss1	Ste12TeSte5Kss1	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{vol} (\text{compartment}) \cdot \text{k22} \cdot [\text{Kss1}] \cdot [\text{Ste12TeSte5}]$$
 (46)

7.23 Reaction v23

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name v23

SBO:0000216 phosphorylation

Reaction equation

$$Ste12TeSte5 \xrightarrow{Kss1PP} Ste12TeSte5P$$
 (47)

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
Ste12TeSte5	Ste12TeSte5	

Table 55: Properties of each modifier.

Id	Name	SBO
Kss1PP	Kss1PP	

Table 56: Properties of each product.

Id	Name	SBO
Ste12TeSte5P	Ste12TeSte5P	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{vol} (\text{compartment}) \cdot \text{k23} \cdot [\text{Ste12TeSte5}] \cdot [\text{Kss1PP}]$$
 (48)

7.24 Reaction v24

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name v24

SBO:0000179 degradation

Reaction equation

$$Ste12TeSte5 \stackrel{Fus3PP}{\longleftarrow} p \tag{49}$$

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
Ste12TeSte5	Ste12TeSte5	

Table 58: Properties of each modifier.

Id	Name	SBO
Fus3PP	Fus3PP	

Table 59: Properties of each product.

Id	Name	SBO
р	p	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \text{vol} (\text{compartment}) \cdot \text{k24} \cdot [\text{Ste12TeSte5}] \cdot [\text{Fus3PP}]$$
 (50)

7.25 Reaction v25

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name v25

SBO:0000205 composite biochemical process

Reaction equation

$$s \xrightarrow{\underline{Ste12TeSte5P}} FREP \tag{51}$$

Reactant

Table 60: Properties of each reactant.

Id	Name	SBO
ន	S	

Table 61: Properties of each modifier.

Id	Name	SBO
Ste12TeSte5P	Ste12TeSte5P	

Table 62: Properties of each product.

Id	Name	SBO
FREP	FREP	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \text{vol} (\text{compartment}) \cdot \text{k25} \cdot [\text{Ste12TeSte5P}]$$
 (52)

7.26 Reaction v26

This is a reversible reaction of one reactant forming one product.

Name v26

SBO:0000330 dephosphorylation

Reaction equation

$$Fus3PP \Longrightarrow Fus3 \tag{53}$$

Reactant

Table 63: Properties of each reactant.

Id	Name	SBO
Fus3PP	Fus3PP	

Product

Table 64: Properties of each product.

Id	Name	SBO
Fus3	Fus3	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \text{vol}\left(\text{compartment}\right) \cdot \text{k26} \cdot [\text{Fus3PP}]$$
 (54)

7.27 Reaction v27

This is a reversible reaction of one reactant forming two products.

Name v27

SBO:0000180 dissociation

Reaction equation

$$Ste5Ste11 \Longrightarrow Ste5 + Ste11 \tag{55}$$

Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
Ste5Ste11	Ste5Ste11	

Products

Table 66: Properties of each product.

Id	Name	SBO
Ste5	Ste5	
Ste11	Ste11	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \text{vol} (\text{compartment}) \cdot \text{k27} \cdot [\text{Ste5Ste11}]$$
 (56)

7.28 Reaction v28

This is a reversible reaction of one reactant forming one product.

Name v28

SBO:0000330 dephosphorylation

Reaction equation

$$Ste12P \Longrightarrow Ste12 \tag{57}$$

Reactant

Table 67: Properties of each reactant.

Id	Name	SBO
Ste12P	Ste12P	

Product

Table 68: Properties of each product.

Id	Name	SBO
Ste12	Ste12	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \text{vol} \left(\text{compartment} \right) \cdot \text{k31} \cdot \left[\text{Ste12P} \right]$$
 (58)

7.29 Reaction v29

This is a reversible reaction of one reactant forming one product.

Name v29

SBO:0000179 degradation

Reaction equation

$$PREP \rightleftharpoons p \tag{59}$$

Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
PREP	PREP	

Table 70: Properties of each product.

Id	Name	SBO
р	p	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \text{vol}(\text{compartment}) \cdot \text{k32} \cdot [\text{PREP}]$$
 (60)

7.30 Reaction v30

This is a reversible reaction of one reactant forming one product.

Name v30

SBO:0000330 dephosphorylation

Reaction equation

$$Ste12TeSte5P \Longrightarrow Ste12TeSte5$$
 (61)

Reactant

Table 71: Properties of each reactant.

Id	Name	SBO
Ste12TeSte5P	Ste12TeSte5P	

Product

Table 72: Properties of each product.

Id	Name	SBO
Ste12TeSte5	Ste12TeSte5	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \text{vol}\left(\text{compartment}\right) \cdot \text{k33} \cdot \left[\text{Ste12TeSte5P}\right]$$
 (62)

7.31 Reaction v31

This is a reversible reaction of one reactant forming one product.

Name v31

SBO:0000179 degradation

Reaction equation

$$FREP \rightleftharpoons p$$
 (63)

Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
FREP	FREP	

Product

Table 74: Properties of each product.

Id	Name	SBO
р	p	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \text{vol}(\text{compartment}) \cdot \text{k34} \cdot [\text{FREP}]$$
 (64)

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 Ste5

Name Ste5

SBO:0000252 polypeptide chain

Initial concentration 42.3 mol·1⁻¹

This species takes part in three reactions (as a reactant in v1, v7 and as a product in v27).

$$\frac{d}{dt}Ste5 = |v_{27}| - |v_1| - |v_7| \tag{65}$$

8.2 Species Ste11

Name Ste11

SBO:0000252 polypeptide chain

Initial concentration $13.3 \text{ mol} \cdot l^{-1}$

This species takes part in four reactions (as a reactant in v1, v13 and as a product in v14, v27).

$$\frac{d}{dt}Ste11 = v_{14} + v_{27} - v_1 - v_{13}$$
 (66)

8.3 Species Ste5Ste11

Name Ste5Ste11

SBO:0000297 protein complex

Initial concentration $5.6 \text{ mol} \cdot l^{-1}$

This species takes part in three reactions (as a reactant in v2, v27 and as a product in v1).

$$\frac{d}{dt}Ste5Ste11 = |v_1| - |v_2| - |v_{27}|$$
 (67)

8.4 Species Gbg

Name Gbg

SBO:0000252 polypeptide chain

Initial concentration $53 \text{ mol} \cdot 1^{-1}$

This species takes part in two reactions (as a reactant in v2 and as a product in v7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gbg} = |v_7| - |v_2| \tag{68}$$

8.5 Species Ste5Ste11Gbg

Name Ste5Ste11Gbg

SBO:0000297 protein complex

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

This species takes part in three reactions (as a reactant in v3, v9 and as a product in v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ste5Ste11Gbg} = |v_2| - |v_3| - |v_9| \tag{69}$$

8.6 Species Fus3

Name Fus3

SBO:0000252 polypeptide chain

Initial concentration $217 \text{ mol} \cdot l^{-1}$

This species takes part in three reactions (as a reactant in v3, v6 and as a product in v26).

$$\frac{d}{dt} Fus3 = |v_{26}| - |v_3| - |v_6| \tag{70}$$

8.7 Species Ste5Ste11GbgFus3

Name Ste5Ste11GbgFus3

SBO:0000297 protein complex

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

This species takes part in two reactions (as a reactant in v4 and as a product in v3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ste5Ste11GbgFus3} = |v_3| - |v_4| \tag{71}$$

8.8 Species Ste5Ste11GbgFus3P

Name Ste5Ste11GbgFus3P

SBO:0000297 protein complex

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

This species takes part in three reactions (as a reactant in v5 and as a product in v4, v6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ste5Ste11GbgFus3P} = v_4 + v_6 - v_5 \tag{72}$$

8.9 Species Fus3PP

Name Fus3PP

SBO:0000252 polypeptide chain

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

This species takes part in five reactions (as a reactant in v26 and as a product in v5 and as a modifier in v16, v19, v24).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fus3PP} = |v_5| - |v_{26}| \tag{73}$$

8.10 Species Ste5Ste11GbgP

Name Ste5Ste11GbgP

SBO:0000297 protein complex

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

This species takes part in five reactions (as a reactant in v6, v7, v12 and as a product in v5, v11).

$$\frac{d}{dt}Ste5Ste11GbgP = v_5 + v_{11} - v_6 - v_7 - v_{12}$$
 (74)

8.11 Species StellUbi

Name Ste11Ubi

SBO:0000252 polypeptide chain

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

This species takes part in three reactions (as a reactant in v8 and as a product in v7 and as a modifier in v15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ste}11\mathrm{Ubi} = |v_7| - |v_8| \tag{75}$$

8.12 Species p

Name p

SBO:0000291 empty set

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

This species takes part in four reactions (as a product in v8, v24, v29, v31), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p} = 0\tag{76}$$

8.13 Species Kss1

Name Kss1

SBO:0000252 polypeptide chain

Initial concentration 54.4 mol·l⁻¹

This species takes part in eight reactions (as a reactant in v9, v12, v15, v18, v22 and as a product in v16, v17, v21).

$$\frac{d}{dt}Kss1 = |v_{16}| + 2|v_{17}| + |v_{21}| - |v_{9}| - |v_{12}| - |v_{15}| - 2|v_{18}| - |v_{22}|$$
(77)

8.14 Species Ste5Ste11GbgKss1

Name Ste5Ste11GbgKss1

SBO:0000297 protein complex

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

This species takes part in two reactions (as a reactant in v10 and as a product in v9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ste5Ste11GbgKss1} = v_9 - v_{10} \tag{78}$$

8.15 Species Ste5Ste11GbgKss1P

Name Ste5Ste11GbgKss1P

SBO:0000297 protein complex

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

This species takes part in three reactions (as a reactant in v11 and as a product in v10, v12).

$$\frac{d}{dt}Ste5Ste11GbgKss1P = |v_{10}| + |v_{12}| - |v_{11}|$$
 (79)

8.16 Species Kss1PP

Name Kss1PP

SBO:0000252 polypeptide chain

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

This species takes part in five reactions (as a reactant in v16 and as a product in v11, v15 and as a modifier in v19, v23).

$$\frac{d}{dt}Kss1PP = |v_{11}| + |v_{15}| - |v_{16}|$$
(80)

8.17 Species Ste11P

Name Ste11P

SBO:0000252 polypeptide chain

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

This species takes part in three reactions (as a reactant in v14 and as a product in v13 and as a modifier in v15).

$$\frac{d}{dt}Ste11P = v_{13} - v_{14}$$
 (81)

8.18 Species Ste12Kss1

Name Ste12Kss1

SBO:0000297 protein complex

Initial concentration $35.9 \text{ mol} \cdot l^{-1}$

This species takes part in two reactions (as a reactant in v17 and as a product in v18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ste}12\mathrm{Kss}1 = |v_{18}| - |v_{17}| \tag{82}$$

8.19 Species Ste12

Name Ste12

SBO:0000252 polypeptide chain

Initial concentration $0.07 \text{ mol} \cdot l^{-1}$

This species takes part in four reactions (as a reactant in v18, v19 and as a product in v17, v28).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ste}12 = |v_{17}| + |v_{28}| - |v_{18}| - |v_{19}| \tag{83}$$

8.20 Species Ste12P

Name Ste12P

SBO:0000252 polypeptide chain

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

This species takes part in three reactions (as a reactant in v28 and as a product in v19 and as a modifier in v20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ste}12\mathrm{P} = |v_{19}| - |v_{28}| \tag{84}$$

8.21 Species s

Name s

SBO:0000291 empty set

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

This species takes part in two reactions (as a reactant in v20, v25), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{s} = 0\tag{85}$$

8.22 Species PREP

Name PREP

SBO:0000406 observable

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

This species takes part in two reactions (as a reactant in v29 and as a product in v20).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{PREP} = |v_{20}| - |v_{29}| \tag{86}$$

8.23 Species Ste12TeSte5Kss1

Name Ste12TeSte5Kss1

SBO:0000297 protein complex

Initial concentration $13.7 \text{ mol} \cdot l^{-1}$

This species takes part in two reactions (as a reactant in v21 and as a product in v22).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ste}12\mathrm{Te}\mathrm{Ste}5\mathrm{Kss}1 = v_{22} - v_{21} \tag{87}$$

8.24 Species Ste12TeSte5

Name Ste12TeSte5

SBO:0000297 protein complex

Initial concentration $0.25 \text{ mol} \cdot l^{-1}$

This species takes part in five reactions (as a reactant in v22, v23, v24 and as a product in v21, v30).

$$\frac{d}{dt}Ste12TeSte5 = v_{21} + v_{30} - v_{22} - v_{23} - v_{24}$$
(88)

8.25 Species Ste12TeSte5P

Name Ste12TeSte5P

SBO:0000297 protein complex

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

This species takes part in three reactions (as a reactant in v30 and as a product in v23 and as a modifier in v25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ste}12\mathrm{Te}\mathrm{Ste}5\mathrm{P} = |v_{23}| - |v_{30}| \tag{89}$$

8.26 Species FREP

Name FREP

SBO:0000406 observable

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

This species takes part in two reactions (as a reactant in v31 and as a product in v25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FREP} = |v_{25}| - |v_{31}| \tag{90}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000177 non-covalent binding: Interaction between several biochemical entities that results in the formation of a non-covalent comple

SBO:0000179 degradation: Complete disappearance of a physical entity

SBO:0000180 dissociation: Transformation of a non-covalent complex that results in the formation of several independent biochemical entitie

- **SBO:0000205 composite biochemical process:** Process that involves the participation of chemical or biological entities and is composed of several elementary steps or reactions.
- **SBO:0000216 phosphorylation:** Addition of a phosphate group (-H2PO4) to a chemical entity
- **SBO:0000252 polypeptide chain:** Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654
- **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:0000291 empty set:** Entity defined by the absence of any actual object. An empty set is often used to represent the source of a creation process or the result of a degradation process.
- **SBO:0000297 protein complex:** Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608
- **SBO:0000330 dephosphorylation:** Removal of a phosphate group (-H2PO4) from a chemical entity.
- **SBO:0000406 observable:** An entity that can be measured quantitativel

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