SBML Model Report

Model name: “Schaber2012 - Hog pathway in yeast”

May 5, 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 Joerg Schaber[2] at November 22nd 2012 at 6:31 p. m. and last time modified at December 14th 2012 at 2:24 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	4
species types	0	species	15
events	0	constraints	0
reactions	16	function definitions	10
global parameters	88	unit definitions	1
rules	22	initial assignments	37

Model Notes

Schaber2012 - Hog pathway in yeast

The high osmolarity glycerol (HOG) pathway in the yeast Saccharomyces cerevisiae is one of the best-studied mitogen-activated protein kinase (MAPK) pathways and serves as a prototype

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signalling system for eukaryotes. This pathway is necessary and sufficient to adapt to high external osmolarity. A key component of this pathway is the stress-activated protein kinase (SAPK) Hog1, which is rapidly phosphorylated by the SAPK kinase Pbs2 upon hyper-osmotic shock, and which is the terminal kinase of two parallel signalling pathways, subsequently called the Sho1 branch and the Sln1 branch, respectively. Ensemble modelling (192 models) is used to study the yeast HOG pathway, a prototype for eukaryotic mitogen-activated kinase signalling systems. The best fit model (Model Nr.22: described here) provides new insights into the function of this system, some of which are then experimentally validated.

This model is described in the article:Modelling reveals novel roles of two parallel signalling pathways and homeostatic feedbacks in yeast.Schaber J, Baltanas R, Bush A, Klipp E, Colman-Lerner A.Mol Syst Biol. 2012 Nov 13;8:622.

Abstract:

The high osmolarity glycerol (HOG) pathway in yeast serves as a prototype signalling system for eukaryotes. We used an unprecedented amount of data to parameterise 192 models capturing different hypotheses about molecular mechanisms underlying osmo-adaptation and selected a best approximating model. This model implied novel mechanisms regulating osmo-adaptation in yeast. The model suggested that (i) the main mechanism for osmo-adaptation is a fast and transient non-transcriptional Hog1-mediated activation of glycerol production, (ii) the transcriptional response serves to maintain an increased steady-state glycerol production with low steady-state Hog1 activity, and (iii) fast negative feedbacks of activated Hog1 on upstream signalling branches serves to stabilise adaptation response. The best approximating model also indicated that homoeostatic adaptive systems with two parallel redundant signalling branches show a more robust and faster response than single-branch systems. We corroborated this notion to a large extent by dedicated measurements of volume recovery in single cells. Our study also demonstrates that systematically testing a model ensemble against data has the potential to achieve a better and unbiased understanding of molecular mechanisms.

This model is hosted on BioModels Database and identified by: MODEL1209110001 .

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models .

2 Unit Definitions

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

2.1 Unit `substance`

Name substance

Definition µmol

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 Compartments

This model contains four compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment_1	Vos		3	29.5	l	☐	
compartment_2	Vex		3	50000	l	☑	
compartment_3	V		3	50	l	☐	
compartment_4	M		3	1	litre	☑	

3.1 Compartment compartment_1

This is a three dimensional compartment with a not constant size of 29.5 litre.

Name Vos

Notes Osmolytically active volume, derived from a total cell volume of 50 fl and a solid

3.2 Compartment compartment_2

This is a three dimensional compartment with a constant size of 50000 litre.

Name Vex

3.3 Compartment compartment_3

This is a three dimensional compartment with a not constant size of 50 litre.

Name V

Notes Total cell volume.

3.4 Compartment compartment_4

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

Name M

4 Species

This model contains 15 species. The boundary condition of one of these species is set to `true` so that this species' amount cannot be changed by any reaction. Section 10 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
species_1	Glyin	compartment_1	µmol	⊟	⊟
species_2	Hog1	compartment_1	µmol	⊟	⊟
species_3	Hog1PP	compartment_1	µmol	⊟	⊟
species_4	Pbs2	compartment_1	µmol	⊟	⊟
species_5	Pbs2P	compartment_1	µmol	⊟	⊟
species_6	Phosphatase	compartment_1	µmol	⊟	⊟
species_7	Protein	compartment_1	µmol	⊟	⊟
species_8	RNA	compartment_1	µmol	⊟	⊟
species_9	Hog1P	compartment_1	µmol	⊟	⊟
species_10	Sho1	compartment_1	µmol	⊟	⊟
species_11	Sho1Pbs2P	compartment_1	µmol	⊟	⊟
species_12	Hog1PPActive	compartment_1	µmol	⊟	☑
species_13	Glyex	compartment_2	µmol	⊟	⊟
species_14	Fps1	compartment_4	µmol	⊟	⊟
species_15	Fps1P	compartment_4	µmol	⊟	⊟

5 Parameters

This model contains 88 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
parameter_1	R		8.314		☑
parameter_2	T		303.150		☑
parameter_3	mol		$6.022 \cdot 10^{23}$		☑
parameter_4	phi		0.930		☑
parameter_5	c2p		10^{-9}		☑
parameter_6	tm		10.000		☑
parameter_7	Lp		0.013		☑
parameter_8	P0		0.610		☑
parameter_9	eps		14.300		☑
parameter_10	minf		0.410		☑
parameter_11	ce_0		260000.000		☑
parameter_12	V_0		50.000		☑
parameter_13	Vb		20.500		☑
parameter_14	maxHog1nucf		0.800		☑
parameter_15	VP_0		47.912		☑
parameter_16	Area		65.634		☐
parameter_17	Hog1PPrelIniwt		2.230		☑
parameter_18	N2uM		$5.62907756305974 \cdot 10^{-5}$		☑
parameter_19	ci_0		502026.122		☑
parameter_20	cin_0		322026.122		☑
parameter_21	Turgor		0.610		☐
parameter_22	ActivationSln1-_nlfb		$7.10539561053171 \cdot 10^{-4}$		☐
parameter_23	NaCl		0.400		☑
parameter_24	ActivOffsetSln1-_nlfb		$-7.10539561053171 \cdot 10^{-4}$		☑
parameter_25	kHog1phos1		42.640		☑
parameter_26	kHog1dephos		1.786		☑
parameter_27	ks		$4.28194136809108 \cdot 10^{-4}$		☐
parameter_28	Fps1TransportCapacitty		0.500		☐
parameter_29	FitVrel		100.000		☐
parameter_30	FitHog1PPrel		2.230		☐
parameter_31	FitProteinrel		19.900		☐
parameter_32	FitGlyinrel		17.000		☐
parameter_33	Turgor2Osm		242026.122		☐
parameter_34	Fps1ClosureRate		0.128		☑
parameter_35	Protein_deg_k		$6.78688610600496 \cdot 10^{-5}$		☑

Id	Name	SBO	Value	Unit	Constant
parameter_36	FitRNArel		3.400		⊟
parameter_37	Hog1Total		0.382		☑
parameter_38	Pbs2Total		0.122		☑
parameter_39	RNA_deg_k_MM		7.096		☑
parameter_40	Sho1Total		0.131		☑
parameter_41	kHog1phos2		48.000		☑
parameter_42	Hog1PPrelIniSln1		2.230		☑
parameter_43	Hog1PPrelIniSho1		2.230		☑
parameter_44	Osmex		260000.000		⊟
parameter_45	Osmin		502026.122		⊟
parameter_46	Vos_0		29.500		☑
parameter_47	A_0		65.634		☑
parameter_48	ts		600.000		☑
parameter_49	cen		258200.000		⊟
parameter_50	Glyex_0		1800.000		☑
parameter_51	Protein_0		0.045		☑
parameter_52	RNA_0		0.034		☑
parameter_53	Glyin_0		180000.000		☑
parameter_54	Hog1PP_0		0.007		☑
parameter_55	ActivOffsetSho1-_nlfb		−0.004		☑
parameter_56	ActivationSho1-_nlfb		0.004		⊟
parameter_57	Sho1BranchActive		1.000		☑
parameter_58	Sln1BranchActive		1.000		☑
parameter_59	Fps1TotalIni		0.051		☑
parameter_60	Fps1TotalTrans		0.051		⊟
parameter_61	TurgorActiv_h		2.000		☑
parameter_62	TurgorActivation		0.500		⊟
parameter_63	TurgorDeactivation		0.500		⊟
parameter_64	v16_5_k		0.003		☑
parameter_65	v16_6_k		0.003		☑
parameter_66	v16_7_k		0.005		☑
parameter_67	Hog1Activity		0.001		☑
parameter_68	tinh		600.000		☑
parameter_69	Hog1Inhibition		1.000		⊟
parameter_70	Inhibition		0.000		☑
parameter_71	Fps1Delta		1.000		☑
parameter_72	v2_k		0.607		☑
parameter_73	v1_fb_Ki		0.009		☑
parameter_74	v1_fb_h		0.346		☑
parameter_75	v1_fb_k		0.075		☑

Id	Name	SBO	Value	Unit	Constant
parameter_76	v11_k		$9.06781 \cdot 10^{-5}$		☑
parameter_77	v9_k		18.182		☑
parameter_78	v9_Km		0.507		☑
parameter_79	v4_k1		0.002		☑
parameter_80	v3_fb_Ki		0.298		☑
parameter_81	v3_fb_h		2.079		☑
parameter_82	v3_fb_k		0.005		☑
parameter_83	v15_5_k		0.005		☑
parameter_84	v16_6_Ki		0.081		☑
parameter_85	v16_6_h		0.629		☑
parameter_86	v13_k1		680.818		☑
parameter_87	v13_k2		46.836		☑
parameter_88	v13_Km		0.421		☑

6 Initialassignments

This is an overview of 37 initialassignments.

6.1 Initialassignment compartment_1

Derived unit contains undeclared units

Math parameter_46

6.2 Initialassignment compartment_2

Derived unit contains undeclared units

Math $1000 \cdot \mathrm{vol}\left(\mathrm{compartment\_3}\right)$

6.3 Initialassignment species_1

Derived unit contains undeclared units

Math $\mathrm{parameter\_53} \cdot \mathrm{vol}\left(\mathrm{compartment\_1}\right)$

6.4 Initialassignment species_2

Derived unit contains undeclared units

Math $\left(\mathrm{parameter\_37} - \frac{\mathrm{species\_9}}{\mathrm{vol}(\mathrm{compartment\_1})} - \frac{\mathrm{species\_3}}{\mathrm{vol}(\mathrm{compartment\_1})}\right) \cdot \mathrm{vol}\left(\mathrm{compartment\_1}\right)$

6.5 Initialassignment species_3

Derived unit contains undeclared units

Math $\text{parameter\_54} \cdot \text{vol}\left(\text{compartment\_1}\right)$

6.6 Initialassignment species_4

Derived unit contains undeclared units

Math $\left(\text{parameter\_38} - \frac{\text{species\_5}}{\text{vol}(\text{compartment\_1})} - \frac{\text{species\_11}}{\text{vol}(\text{compartment\_1})}\right) \cdot \text{vol}\left(\text{compartment\_1}\right)$

6.7 Initialassignment species_5

Derived unit contains undeclared units

Math $$\begin{cases} \left(\frac{\text{parameter\_26} \cdot \frac{\text{species\_6}}{\text{vol}(\text{compartment\_1})} \cdot \left(\frac{\text{species\_3}}{\text{vol}(\text{compartment\_1})} + \sqrt{2}\right)}{4 \cdot \text{parameter\_25} \cdot \left(\frac{\text{species\_3}}{\text{vol}(\text{compartment\_1})} - \text{parameter\_37}\right)}\right) & \\ \begin{cases} \left(\frac{\text{parameter\_25} \cdot \text{parameter\_26} \cdot \frac{\text{species\_6}}{\text{vol}(\text{compartment\_1})} \cdot \frac{\text{species\_3}}{\text{vol}(\text{compartment\_1})} + \sqrt{2}}{2 \cdot \text{parameter\_25}^2 \cdot \left(\frac{\text{species\_3}}{\text{vol}(\text{compartment\_1})} - \text{parameter\_37}\right)}\right) & \text{if } (\text{parameter\_58} = 1) \wedge (\text{para} \\ 0 & \text{otherwise} \end{cases} \end{cases} \text{vol}\left(\text{compartment\_1}\right)$$

6.8 Initialassignment species_6

Derived unit contains undeclared units

Math $769 \cdot \text{parameter\_18} \cdot \text{vol}\left(\text{compartment\_1}\right)$

6.9 Initialassignment species_7

Derived unit contains undeclared units

Math $\text{parameter\_51} \cdot \text{vol}\left(\text{compartment\_1}\right)$

6.10 Initialassignment species_8

Derived unit contains undeclared units

Math $\text{parameter\_52} \cdot \text{vol}\left(\text{compartment\_1}\right)$

6.11 Initialassignment species_9

Derived unit contains undeclared units

Math
$$\frac{\begin{cases} \frac{1}{2}\cdot\left(\left(\frac{\text{species\_3}}{\text{vol}\left(\text{compartment\_1}\right)}\right)+\sqrt{2}\right) & \\ \begin{cases} \frac{\text{parameter\_25}\cdot\text{parameter\_26}\cdot\frac{\text{species\_6}}{\text{vol}\left(\text{compartment\_1}\right)}\cdot\frac{\text{species\_3}}{\text{vol}\left(\text{compartment\_1}\right)}+\sqrt{2}}{2\cdot\text{parameter\_25}\cdot\text{parameter\_26}\cdot\frac{\text{species\_6}}{\text{vol}\left(\text{compartment\_1}\right)}} & \text{if } \left(\text{parameter\_58}=1\right)\wedge\left(\text{paramete}\right. \\ \frac{\text{parameter\_41}\cdot\text{parameter\_26}\cdot\frac{\text{species\_6}}{\text{vol}\left(\text{compartment\_1}\right)}\cdot\frac{\text{species\_3}}{\text{vol}\left(\text{compartment\_1}\right)}+\sqrt{2}}{2\cdot\text{parameter\_41}\cdot\text{parameter\_26}\cdot\frac{\text{species\_6}}{\text{vol}\left(\text{compartment\_1}\right)}} & \text{otherwise} \end{cases} & \end{cases}}{\text{vol}\left(\text{compartment\_1}\right)}$$

6.12 Initialassignment species_10

Derived unit contains undeclared units

Math
$$\left(\text{parameter\_40}-\frac{\text{species\_11}}{\text{vol}\left(\text{compartment\_1}\right)}\right)\cdot\text{vol}\left(\text{compartment\_1}\right)$$

6.13 Initialassignment species_11

Derived unit contains undeclared units

Math
$$\frac{\begin{cases} \left(\frac{\text{parameter\_26}\cdot\frac{\text{species\_6}}{\text{vol}\left(\text{compartment\_1}\right)}\cdot\left(\frac{\text{species\_3}}{\text{vol}\left(\text{compartment\_1}\right)}+\sqrt{2}\right)}{4\cdot\text{parameter\_41}\cdot\left(\frac{\text{species\_3}}{\text{vol}\left(\text{compartment\_1}\right)}-\text{parameter\_37}\right)}\right) & \\ \begin{cases} \left(\frac{\text{parameter\_41}\cdot\text{parameter\_26}\cdot\frac{\text{species\_6}}{\text{vol}\left(\text{compartment\_1}\right)}\cdot\frac{\text{species\_3}}{\text{vol}\left(\text{compartment\_1}\right)}+\sqrt{2}}{2\cdot\text{parameter\_41}^2\cdot\left(\frac{\text{species\_3}}{\text{vol}\left(\text{compartment\_1}\right)}-\text{parameter\_37}\right)}\right) & \text{if } \left(\text{parameter\_58}=0\right)\wedge\left(\text{para}\right. \\ 0 & \text{otherwise} \end{cases} & \end{cases}}{\text{vol}\left(\text{compartment\_1}\right)}$$

6.14 Initialassignment species_13

Derived unit contains undeclared units

Math
$$\frac{\frac{\text{species\_1}}{\text{vol}\left(\text{compartment\_1}\right)}}{100}\cdot\text{vol}\left(\text{compartment\_2}\right)$$

6.15 Initialassignment species_14

Derived unit contains undeclared units

Math
$$\frac{\text{parameter\_59}}{2}\cdot\text{vol}\left(\text{compartment\_4}\right)$$

6.16 Initialassignment species_15

Derived unit contains undeclared units

Math $\frac{\text{parameter\_59}}{2} \cdot \text{vol}\left(\text{compartment\_4}\right)$

6.17 Initialassignment parameter_13

Derived unit contains undeclared units

Math $\text{parameter\_12} \cdot \text{parameter\_10}$

6.18 Initialassignment parameter_15

Derived unit contains undeclared units

Math $\text{parameter\_12} \cdot \exp\left(\frac{\text{parameter\_8}}{\text{parameter\_9}}\right)$

6.19 Initialassignment parameter_18

Derived unit contains undeclared units

Math $\frac{1.0E21}{\text{parameter\_3} \cdot \text{vol}(\text{compartment\_1})}$

6.20 Initialassignment parameter_19

Derived unit contains undeclared units

Math $\text{parameter\_11} + \frac{\text{parameter\_8}}{\text{parameter\_5} \cdot \text{parameter\_1} \cdot \text{parameter\_2}}$

6.21 Initialassignment parameter_20

Derived unit contains undeclared units

Math $\text{parameter\_19} - \frac{\text{species\_1}}{\text{vol}(\text{compartment\_1})}$

6.22 Initialassignment parameter_24

Derived unit contains undeclared units

Math $\frac{\text{parameter\_72} \cdot \frac{\text{species\_6}}{\text{vol}(\text{compartment\_1})} \cdot \frac{\text{species\_5}}{\text{vol}(\text{compartment\_1})} \cdot \left(1 + \left(\frac{\frac{\text{species\_3}}{\text{vol}(\text{compartment\_1})}}{\text{parameter\_73}}\right)^{\text{parameter\_74}}\right)}{\text{parameter\_75} \cdot \frac{\text{species\_4}}{\text{vol}(\text{compartment\_1})}}$

6.23 Initialassignment parameter_35

Derived unit contains undeclared units

Math $\frac{\text{parameter\_76} \cdot \frac{\text{species\_8}}{\text{vol(compartment\_1)}}}{\frac{\text{species\_7}}{\text{vol(compartment\_1)}}}$

6.24 Initialassignment parameter_37

Derived unit contains undeclared units

Math $6788 \cdot \text{parameter\_18}$

6.25 Initialassignment parameter_38

Derived unit contains undeclared units

Math $2160 \cdot \text{parameter\_18}$

6.26 Initialassignment parameter_39

Derived unit contains undeclared units

Math $\frac{\frac{\text{parameter\_77} \cdot \frac{\text{species\_3}}{\text{vol(compartment\_1)}}}{\text{parameter\_78} + \frac{\text{species\_3}}{\text{vol(compartment\_1)}}}}{\frac{\text{species\_8}}{\text{vol(compartment\_1)}}}$

6.27 Initialassignment parameter_40

Derived unit contains undeclared units

Math $2330 \cdot \text{parameter\_18}$

6.28 Initialassignment parameter_46

Derived unit contains undeclared units

Math $\text{parameter\_12} \cdot (1 - \text{parameter\_10})$

6.29 Initialassignment parameter_47

Derived unit contains undeclared units

Math $(36 \cdot \pi)^{\frac{1}{3}} \cdot \text{parameter\_12}^{\frac{2}{3}}$

6.30 Initialassignment parameter_50

Derived unit contains undeclared units

Math $\frac{\text{parameter\_53}}{100}$

6.31 Initialassignment parameter_51

Derived unit contains undeclared units

Math $807 \cdot \text{parameter\_18}$

6.32 Initialassignment parameter_54

Derived unit contains undeclared units

Math
$$\begin{cases} \dfrac{\text{parameter\_37} \cdot \text{parameter\_17} \cdot \text{parameter\_14}}{100} & \text{if } (\text{paramete} \\ \begin{cases} \dfrac{\text{parameter\_37} \cdot \text{parameter\_42} \cdot \text{parameter\_14}}{100} & \text{if } (\text{parameter\_58} = 1) \wedge (\text{parameter\_57} = 0) \\ \dfrac{\text{parameter\_37} \cdot \text{parameter\_43} \cdot \text{parameter\_14}}{100} & \text{otherwise} \end{cases} & \text{otherwise} \end{cases}$$

6.33 Initialassignment parameter_55

Derived unit contains undeclared units

Math
$$\frac{\text{parameter\_79} \cdot \frac{\text{species\_11}}{\text{vol(compartment\_1)}} \cdot \left(1 + \left(\frac{\frac{\text{species\_3}}{\text{vol(compartment\_1)}}}{\text{parameter\_80}}\right)^{\text{parameter\_81}}\right)}{\text{parameter\_82} \cdot \frac{\text{species\_4}}{\text{vol(compartment\_1)}} \cdot \frac{\text{species\_10}}{\text{vol(compartment\_1)}}}$$

6.34 Initialassignment parameter_59

Derived unit contains undeclared units

Math $907 \cdot \text{parameter\_18}$

6.35 Initialassignment parameter_64

Derived unit contains undeclared units

Math
$$\frac{\text{parameter\_83} \cdot \frac{\text{species\_14}}{\text{vol(compartment\_4)}} \cdot \text{parameter\_63}}{\frac{\text{species\_15}}{\text{vol(compartment\_4)}}}$$

6.36 Initialassignment parameter_65

Derived unit contains undeclared units

Math
$$\frac{\text{parameter\_83} \cdot \frac{\text{species\_14}}{\text{vol(compartment\_4)}} \cdot \text{parameter\_63} \cdot \left(1 + \left(\frac{\frac{\text{species\_3}}{\text{vol(compartment\_1)}}}{\text{parameter\_84}}\right)^{\text{parameter\_85}}\right)}{\frac{\text{species\_15}}{\text{vol(compartment\_4)}}}$$

6.37 Initialassignment parameter_66

Derived unit contains undeclared units

Math $\frac{\text{parameter\_83} \cdot \frac{\text{species\_14}}{\text{vol(compartment\_4)}} \cdot \text{parameter\_63}}{\frac{\text{species\_15}}{\text{vol(compartment\_4)}} \cdot \text{parameter\_62}}$

7 Function definitions

This is an overview of ten function definitions.

7.1 Function definition function_10

Name 1 para inh Mass action (rrev)

Arguments ko, k, S, M, Ki, h

Mathematical Expression

$$\frac{\text{ko} \cdot \text{k} \cdot \text{S}}{1 + \left(\frac{\text{M}}{\text{Ki}}\right)^{\text{h}}} \tag{1}$$

7.2 Function definition function_9

Name 3 param mass action (irrev)

Arguments ko, k, M, S

Mathematical Expression

$$\text{ko} \cdot \text{k} \cdot \text{M} \cdot \text{S} \tag{2}$$

7.3 Function definition function_8

Name 2 param 2 S MA with inhibition (irrev)

Arguments ko, k, M1, S1, S2, M2, Ki, h

Mathematical Expression

$$\frac{\text{ko} \cdot \text{k} \cdot \text{M1} \cdot \text{S1} \cdot \text{S2}}{1 + \left(\frac{\text{M2}}{\text{Ki}}\right)^{\text{h}}} \tag{3}$$

7.4 Function definition function_4

Name Modified constant flux (irrev)

Arguments k, M

Mathematical Expression

$$\text{k} \cdot \text{M} \tag{4}$$

7.5 Function definition function_6

Name transport (rev)

Arguments A, P, S, f, ks

Mathematical Expression

$$f \cdot ks \cdot A \cdot (S - P) \tag{5}$$

7.6 Function definition function_2

Name Modified mass action (irrev)

Arguments k, M, S

Mathematical Expression

$$k \cdot M \cdot S \tag{6}$$

7.7 Function definition function_5

Name 2 param mod. add. constant flux MM (irrev)

Arguments k1, M1, k2, M2, Km

Mathematical Expression

$$\frac{k1 \cdot M1 \cdot (1 + k2 \cdot M2)}{Km + M1 \cdot (1 + k2 \cdot M2)} \tag{7}$$

7.8 Function definition function_7

Name mod. constat flux (MM) (irrev)

Arguments k, M, Km

Mathematical Expression

$$\frac{k \cdot M}{Km + M} \tag{8}$$

7.9 Function definition function_3

Name mod. MA OR (irrev)

Arguments k1, M1, S, k2, M2

Mathematical Expression

$$k1 \cdot M1 \cdot S + k2 \cdot M2 \cdot S \tag{9}$$

7.10 Function definition function_1

Name 3 param activation with inhibition (iirev)

Arguments ko, k, M1, S, M2, h, Ki

Mathematical Expression

$$\frac{\mathrm{ko} \cdot \mathrm{k} \cdot \mathrm{M1} \cdot \mathrm{S}}{1 + \left(\frac{\mathrm{M2}}{\mathrm{Ki}}\right)^{\mathrm{h}}} \tag{10}$$

8 Rules

This is an overview of 22 rules.

8.1 Rule compartment_3

Rule compartment_3 is an assignment rule for compartment compartment_3:

$$\mathrm{vol}\left(\mathrm{compartment\_3}\right) = \mathrm{parameter\_13} + \mathrm{vol}\left(\mathrm{compartment\_1}\right) \tag{11}$$

8.2 Rule parameter_16

Rule parameter_16 is an assignment rule for parameter parameter_16:

$$\mathrm{parameter\_16} = (36 \cdot \pi)^{\frac{1}{3}} \cdot \mathrm{vol}\left(\mathrm{compartment\_3}\right)^{\frac{2}{3}} \tag{12}$$

8.3 Rule parameter_21

Rule parameter_21 is an assignment rule for parameter parameter_21:

$$\mathrm{parameter\_21} = \begin{cases} \mathrm{parameter\_9} \cdot \left(\dfrac{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}{\mathrm{parameter\_15}}\right) & \text{if } \mathrm{vol}\left(\mathrm{compartment\_3}\right) > \mathrm{parameter\_15} \\ 0 & \text{otherwise} \end{cases} \tag{13}$$

8.4 Rule parameter_22

Rule parameter_22 is an assignment rule for parameter parameter_22:

$$\mathrm{parameter\_22} = \begin{cases} \dfrac{\mathrm{parameter\_47} - \mathrm{parameter\_16}}{\mathrm{parameter\_47}} - \mathrm{parameter\_24} & \text{if } \dfrac{\mathrm{parameter\_47} - \mathrm{parameter\_16}}{\mathrm{parameter\_47}} > \mathrm{parameter\_24} \\ 0 & \text{otherwise} \end{cases} \tag{14}$$

8.5 Rule parameter_27

Rule parameter_27 is an assignment rule for parameter parameter_27:

$$\text{parameter\_27} = \frac{\frac{\text{parameter\_86}\cdot\text{parameter\_51}\cdot(1+\text{parameter\_87}\cdot\text{parameter\_54})}{\text{parameter\_88}+\text{parameter\_51}\cdot(1+\text{parameter\_87}\cdot\text{parameter\_54})}\cdot\text{parameter\_46}}{0.5\cdot\text{parameter\_47}\cdot(\text{parameter\_53}-\text{parameter\_50})} \tag{15}$$

8.6 Rule parameter_28

Rule parameter_28 is an assignment rule for parameter parameter_28:

$$\text{parameter\_28} = \frac{\frac{\text{species\_14}}{\text{vol}(\text{compartment\_4})}}{\text{parameter\_59}} \tag{16}$$

8.7 Rule parameter_29

Rule parameter_29 is an assignment rule for parameter parameter_29:

$$\text{parameter\_29} = \frac{100\cdot\text{vol}\,(\text{compartment\_3})}{\text{parameter\_12}} \tag{17}$$

8.8 Rule parameter_30

Rule parameter_30 is an assignment rule for parameter parameter_30:

$$\text{parameter\_30} = \frac{100\cdot\frac{\text{species\_3}}{\text{vol}(\text{compartment\_1})}\cdot\text{vol}\,(\text{compartment\_1})}{\text{parameter\_14}\cdot\text{parameter\_37}\cdot\text{parameter\_46}} \tag{18}$$

8.9 Rule parameter_31

Rule parameter_31 is an assignment rule for parameter parameter_31:

$$\text{parameter\_31} = \frac{19.9\cdot\frac{\text{species\_7}}{\text{vol}(\text{compartment\_1})}\cdot\text{vol}\,(\text{compartment\_1})}{\text{parameter\_51}\cdot\text{parameter\_46}} \tag{19}$$

8.10 Rule parameter_32

Rule parameter_32 is an assignment rule for parameter parameter_32:

$$\text{parameter\_32} = \frac{17\cdot\frac{\text{species\_1}}{\text{vol}(\text{compartment\_1})}\cdot\text{vol}\,(\text{compartment\_1})}{\text{parameter\_53}\cdot\text{parameter\_46}} \tag{20}$$

8.11 Rule parameter_33

Rule parameter_33 is an assignment rule for parameter parameter_33:

$$\text{parameter\_33} = \frac{\text{parameter\_21}}{\text{parameter\_1}\cdot\text{parameter\_2}\cdot\text{parameter\_5}} \tag{21}$$

8.12 Rule parameter_36

Rule parameter_36 is an assignment rule for parameter parameter_36:

$$\text{parameter\_36} = \frac{3.4 \cdot \frac{\text{species\_8}}{\text{vol}(\text{compartment\_1})} \cdot \text{vol}\left(\text{compartment\_1}\right)}{\text{parameter\_52} \cdot \text{parameter\_46}} \tag{22}$$

8.13 Rule parameter_45

Rule parameter_45 is an assignment rule for parameter parameter_45:

$$\text{parameter\_45} = \frac{\text{species\_1}}{\text{vol}\left(\text{compartment\_1}\right)} + \frac{\text{parameter\_20} \cdot \text{parameter\_46}}{\text{vol}\left(\text{compartment\_1}\right)} \tag{23}$$

8.14 Rule parameter_49

Rule parameter_49 is an assignment rule for parameter parameter_49:

$$\text{parameter\_49} \tag{24}$$
$$= \begin{cases} \text{parameter\_11} - \text{parameter\_50} + \left(1 - \exp\left(\frac{\text{parameter\_48} - \text{time}}{\text{parameter\_6}}\right)\right) \cdot 2 \cdot \text{parameter\_4} \cdot \text{parameter\_23} \cdot 10^6 & \text{if} \\ \text{parameter\_11} - \text{parameter\_50} & \text{ot} \end{cases}$$

8.15 Rule parameter_44

Rule parameter_44 is an assignment rule for parameter parameter_44:

$$\text{parameter\_44} = \text{parameter\_49} + \frac{\text{species\_13}}{\text{vol}\left(\text{compartment\_2}\right)} \tag{25}$$

8.16 Rule parameter_56

Rule parameter_56 is an assignment rule for parameter parameter_56:

$$\text{parameter\_56} \tag{26}$$
$$= \begin{cases} \frac{\text{parameter\_47} - \text{parameter\_16}}{\text{parameter\_47}} - \text{parameter\_55} & \text{if } \frac{\text{parameter\_47} - \text{parameter\_16}}{\text{parameter\_47}} > \text{parameter\_55} \\ 0 & \text{otherwise} \end{cases}$$

8.17 Rule parameter_60

Rule parameter_60 is an assignment rule for parameter parameter_60:

$$\text{parameter\_60} = \frac{\text{species\_14}}{\text{vol}\left(\text{compartment\_4}\right)} + \frac{\text{species\_15}}{\text{vol}\left(\text{compartment\_4}\right)} \tag{27}$$

Derived unit $\mu\text{mol} \cdot \text{l}^{-1}$

8.18 Rule parameter_62

Rule parameter_62 is an assignment rule for parameter parameter_62:

$$\text{parameter\_62} = \frac{\text{parameter\_21}^{\text{parameter\_61}}}{\text{parameter\_8}^{\text{parameter\_61}} + \text{parameter\_21}^{\text{parameter\_61}}} \tag{28}$$

8.19 Rule parameter_63

Rule parameter_63 is an assignment rule for parameter parameter_63:

$$\text{parameter\_63} = 1 - \frac{\text{parameter\_21}^{\text{parameter\_61}}}{\text{parameter\_8}^{\text{parameter\_61}} + \text{parameter\_21}^{\text{parameter\_61}}} \tag{29}$$

8.20 Rule parameter_69

Rule parameter_69 is an assignment rule for parameter parameter_69:

$$\text{parameter\_69} = \begin{cases} \begin{cases} \text{parameter\_67} & \text{if time} > \text{parameter\_68} \\ 1 & \text{otherwise} \end{cases} & \text{if parameter\_70} = 1 \\ 1 & \text{otherwise} \end{cases} \tag{30}$$

8.21 Rule species_12

Rule species_12 is an assignment rule for species species_12:

$$[\text{species\_12}] = \text{parameter\_69} \cdot \frac{\text{species\_3}}{\text{vol}\left(\text{compartment\_1}\right)} \cdot \text{vol}\left(\text{compartment\_1}\right) \tag{31}$$

8.22 Rule compartment_1

Rule compartment_1 is a rate rule for compartment compartment_1:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\text{vol}\left(\text{compartment\_1}\right) = {} & \text{parameter\_7} \cdot \text{parameter\_16} \cdot \left(\text{parameter\_21} + \text{parameter\_5}\right. \\ & \left. \cdot\, \text{parameter\_1} \cdot \text{parameter\_2} \cdot \left(\text{parameter\_44} - \text{parameter\_45}\right)\right) \end{aligned} \tag{32}$$

9 Reactions

This model contains 16 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	reaction_1	v1_fb	$\text{species\_4} \xrightarrow{\text{species\_12, species\_4, species\_12}} \text{species\_5}$	
2	reaction_2	v2	$\text{species\_5} \xrightarrow{\text{species\_6, species\_6, species\_5}} \text{species\_4}$	
3	reaction_3	v5	$\text{species\_2} \xrightarrow{\text{species\_5, species\_11, species\_5, species\_2, species\_11}} \text{species\_9}$	
4	reaction_4	v6	$\text{species\_9} \xrightarrow{\text{species\_6, species\_6, species\_9}} \text{species\_2}$	
5	reaction_5	v11	$\emptyset \xrightarrow{\text{species\_8, species\_8}} \text{species\_7}$	
6	reaction_6	v12	$\text{species\_7} \xrightarrow{\text{species\_7}} \emptyset$	
7	reaction_7	v13	$\emptyset \xrightarrow{\text{species\_7, species\_12, species\_7, species\_12}} \text{species\_1}$	
8	reaction_8	v14	$\text{species\_1} \xrightleftharpoons{\text{species\_13, species\_1}} \text{species\_13}$	
9	reaction_9	v9	$\emptyset \xrightarrow{\text{species\_12, species\_12}} \text{species\_8}$	
10	reaction_10	v10	$\text{species\_8} \xrightarrow{\text{species\_8}} \emptyset$	
11	reaction_11	v7	$\text{species\_9} \xrightarrow{\text{species\_5, species\_11, species\_5, species\_9, species\_11}} \text{species\_3}$	
12	reaction_12	v8	$\text{species\_3} \xrightarrow{\text{species\_6, species\_6, species\_3}} \text{species\_9}$	
13	reaction_13	v4	$\text{species\_11} \xrightarrow{\text{species\_11}} \text{species\_10} + \text{species\_4}$	
14	reaction_14	v3_fb	$\text{species\_4} + \text{species\_10} \xrightarrow{\text{species\_12, species\_4, species\_10, species\_12}} \text{species\_11}$	
15	reaction_15	v15_5	$\text{species\_14} \xrightarrow{\text{species\_14}} \text{species\_15}$	

№	Id	Name	Reaction Equation	SBO
16	`reaction_16`	v16_6	species_15 $\xrightarrow{\text{species\_12, species\_15, species\_12}}$ species_14	

9.1 Reaction reaction_1

This is an irreversible reaction of one reactant forming one product influenced by three modifiers.

Name v1_fb

Notes Simple cell surface area dependent linear activation of Pbs2 through the Sln1 branc

Reaction equation

$$\text{species\_4} \xrightarrow{\text{species\_12, species\_4, species\_12}} \text{species\_5} \tag{33}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
species_4	Pbs2	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
species_12	Hog1PPActive	
species_4	Pbs2	
species_12	Hog1PPActive	

Product

Table 8: Properties of each product.

Id	Name	SBO
species_5	Pbs2P	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_1}\left(\mathrm{parameter\_58}, \mathrm{parameter\_75}, \mathrm{parameter\_22}, \frac{\mathrm{species\_4}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \frac{\mathrm{species\_12}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \mathrm{parameter\_74}, \mathrm{parameter\_73}\right) \tag{34}$$

$$\mathrm{function\_1}\left(\mathrm{ko}, \mathrm{k}, \mathrm{M1}, \mathrm{S}, \mathrm{M2}, \mathrm{h}, \mathrm{Ki}\right) = \frac{\mathrm{ko} \cdot \mathrm{k} \cdot \mathrm{M1} \cdot \mathrm{S}}{1 + \left(\frac{\mathrm{M2}}{\mathrm{Ki}}\right)^{\mathrm{h}}} \tag{35}$$

$$\mathrm{function\_1}\left(\mathrm{ko}, \mathrm{k}, \mathrm{M1}, \mathrm{S}, \mathrm{M2}, \mathrm{h}, \mathrm{Ki}\right) = \frac{\mathrm{ko} \cdot \mathrm{k} \cdot \mathrm{M1} \cdot \mathrm{S}}{1 + \left(\frac{\mathrm{M2}}{\mathrm{Ki}}\right)^{\mathrm{h}}} \tag{36}$$

9.2 Reaction `reaction_2`

This is an irreversible reaction of one reactant forming one product influenced by three modifiers.

Name v2

Notes `Constitutive phosphatase dependent deactivation.`

Reaction equation

$$\mathrm{species\_5} \xrightarrow{\mathrm{species\_6,\ species\_6,\ species\_5}} \mathrm{species\_4} \tag{37}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
`species_5`	Pbs2P	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
`species_6`	Phosphatase	
`species_6`	Phosphatase	
`species_5`	Pbs2P	

Product

Table 11: Properties of each product.

Id	Name	SBO
species_4	Pbs2	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_2}\left(\mathrm{parameter\_72}, \frac{\mathrm{species\_6}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \frac{\mathrm{species\_5}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}\right) \tag{38}$$

$$\mathrm{function\_2}\left(\mathrm{k}, \mathrm{M}, \mathrm{S}\right) = \mathrm{k} \cdot \mathrm{M} \cdot \mathrm{S} \tag{39}$$

$$\mathrm{function\_2}\left(\mathrm{k}, \mathrm{M}, \mathrm{S}\right) = \mathrm{k} \cdot \mathrm{M} \cdot \mathrm{S} \tag{40}$$

9.3 Reaction reaction_3

This is an irreversible reaction of one reactant forming one product influenced by five modifiers.

Name v5

Notes Linear phosphorylation of Hog1 by either the scaffold complex (Sho1-branch) or acti

Reaction equation

$$\mathrm{species\_2} \xrightarrow{\mathrm{species\_5},\ \mathrm{species\_11},\ \mathrm{species\_5},\ \mathrm{species\_2},\ \mathrm{species\_11}} \mathrm{species\_9} \tag{41}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
species_2	Hog1	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
species_5	Pbs2P	
species_11	Sho1Pbs2P	
species_5	Pbs2P	
species_2	Hog1	
species_11	Sho1Pbs2P	

Product

Table 14: Properties of each product.

Id	Name	SBO
species_9	Hog1P	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_3}\left(\mathrm{parameter\_25}, \frac{\mathrm{species\_5}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \frac{\mathrm{species\_2}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \mathrm{parameter\_41}, \frac{\mathrm{species\_11}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}\right) \tag{42}$$

$$\mathrm{function\_3}\left(\mathrm{k1}, \mathrm{M1}, \mathrm{S}, \mathrm{k2}, \mathrm{M2}\right) = \mathrm{k1} \cdot \mathrm{M1} \cdot \mathrm{S} + \mathrm{k2} \cdot \mathrm{M2} \cdot \mathrm{S} \tag{43}$$

$$\mathrm{function\_3}\left(\mathrm{k1}, \mathrm{M1}, \mathrm{S}, \mathrm{k2}, \mathrm{M2}\right) = \mathrm{k1} \cdot \mathrm{M1} \cdot \mathrm{S} + \mathrm{k2} \cdot \mathrm{M2} \cdot \mathrm{S} \tag{44}$$

9.4 Reaction reaction_4

This is an irreversible reaction of one reactant forming one product influenced by three modifiers.

Name v6

Notes Constitutive phosphatase dependent de-phosphorylation.

Reaction equation

$$\mathrm{species\_9} \xrightarrow{\mathrm{species\_6,\ species\_6,\ species\_9}} \mathrm{species\_2} \tag{45}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
species_9	Hog1P	

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
species_6	Phosphatase	
species_6	Phosphatase	
species_9	Hog1P	

Product

Table 17: Properties of each product.

Id	Name	SBO
species_2	Hog1	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_2}\left(\mathrm{parameter\_26}, \frac{\mathrm{species\_6}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \frac{\mathrm{species\_9}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}\right) \tag{46}$$

$$\mathrm{function\_2}\left(\mathrm{k}, \mathrm{M}, \mathrm{S}\right) = \mathrm{k} \cdot \mathrm{M} \cdot \mathrm{S} \tag{47}$$

$$\mathrm{function\_2}\left(\mathrm{k}, \mathrm{M}, \mathrm{S}\right) = \mathrm{k} \cdot \mathrm{M} \cdot \mathrm{S} \tag{48}$$

9.5 Reaction reaction_5

This is an irreversible reaction of no reactant forming one product influenced by two modifiers.

Name v11

Notes Protein/enzyme production/synthesis

Reaction equation

$$\emptyset \xrightarrow{\mathrm{species\_8,\ species\_8}} \mathrm{species\_7} \tag{49}$$

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
species_8	RNA	
species_8	RNA	

Product

Table 19: Properties of each product.

Id	Name	SBO
species_7	Protein	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_4}\left(\mathrm{parameter\_76}, \frac{\mathrm{species\_8}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}\right) \tag{50}$$

$$\mathrm{function\_4}\left(\mathrm{k}, \mathrm{M}\right) = \mathrm{k} \cdot \mathrm{M} \tag{51}$$

$$\mathrm{function\_4}\left(\mathrm{k}, \mathrm{M}\right) = \mathrm{k} \cdot \mathrm{M} \tag{52}$$

9.6 Reaction reaction_6

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name v12

Notes Protein/enzyme degradation

Reaction equation

$$\mathrm{species\_7} \xrightarrow{\mathrm{species\_7}} \emptyset \tag{53}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
species_7	Protein	

Modifier

Table 21: Properties of each modifier.

Id	Name	SBO
species_7	Protein	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{parameter\_35} \cdot \text{species\_7} \tag{54}$$

9.7 Reaction reaction_7

This is an irreversible reaction of no reactant forming one product influenced by four modifiers.

Name v13

Notes Glycerol production. As glycerol concentration also involves other proteins and co

Reaction equation

$$\emptyset \xrightarrow{\text{species\_7, species\_12, species\_7, species\_12}} \text{species\_1} \tag{55}$$

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
species_7	Protein	
species_12	Hog1PPActive	
species_7	Protein	
species_12	Hog1PPActive	

Product

Table 23: Properties of each product.

Id	Name	SBO
species_1	Glyin	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_5}\left(\mathrm{parameter\_86}, \frac{\mathrm{species\_7}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \mathrm{parameter\_87}, \frac{\mathrm{species\_12}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \mathrm{parameter\_88}\right) \tag{56}$$

$$\mathrm{function\_5}\left(\mathrm{k1}, \mathrm{M1}, \mathrm{k2}, \mathrm{M2}, \mathrm{Km}\right) = \frac{\mathrm{k1} \cdot \mathrm{M1} \cdot \left(1 + \mathrm{k2} \cdot \mathrm{M2}\right)}{\mathrm{Km} + \mathrm{M1} \cdot \left(1 + \mathrm{k2} \cdot \mathrm{M2}\right)} \tag{57}$$

$$\mathrm{function\_5}\left(\mathrm{k1}, \mathrm{M1}, \mathrm{k2}, \mathrm{M2}, \mathrm{Km}\right) = \frac{\mathrm{k1} \cdot \mathrm{M1} \cdot \left(1 + \mathrm{k2} \cdot \mathrm{M2}\right)}{\mathrm{Km} + \mathrm{M1} \cdot \left(1 + \mathrm{k2} \cdot \mathrm{M2}\right)} \tag{58}$$

9.8 Reaction reaction_8

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

Name v14

Notes Gradient driven glycerol flow out of the cell, where k_tr characterises the state o

Reaction equation

$$\mathrm{species\_1} \xrightleftharpoons{\mathrm{species\_13},\ \mathrm{species\_1}} \mathrm{species\_13} \tag{59}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
species_1	Glyin	

Modifiers

Table 25: Properties of each modifier.

Id	Name	SBO
species_13	Glyex	
species_1	Glyin	

Product

Table 26: Properties of each product.

Id	Name	SBO
species_13	Glyex	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{function\_6}\left(\text{parameter\_16}, \frac{\text{species\_13}}{\text{vol}\left(\text{compartment\_2}\right)}, \frac{\text{species\_1}}{\text{vol}\left(\text{compartment\_1}\right)}, \text{parameter\_28}, \text{parameter\_27}\right) \tag{60}$$

$$\text{function\_6}\left(\text{A}, \text{P}, \text{S}, \text{f}, \text{ks}\right) = \text{f} \cdot \text{ks} \cdot \text{A} \cdot \left(\text{S} - \text{P}\right) \tag{61}$$

9.9 Reaction reaction_9

This is an irreversible reaction of no reactant forming one product influenced by two modifiers.

Name v9

Notes `Gene transcription. Hog1 mediated transcription also involves other proteins that a`

Reaction equation

$$\emptyset \xrightarrow{\text{species\_12, species\_12}} \text{species\_8} \tag{62}$$

Modifiers

Table 27: Properties of each modifier.

Id	Name	SBO
species_12	Hog1PPActive	
species_12	Hog1PPActive	

Product

Table 28: Properties of each product.

Id	Name	SBO
species_8	RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_7}\left(\mathrm{parameter\_77}, \frac{\mathrm{species\_12}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \mathrm{parameter\_78}\right) \tag{63}$$

$$\mathrm{function\_7}\left(\mathrm{k}, \mathrm{M}, \mathrm{Km}\right) = \frac{\mathrm{k} \cdot \mathrm{M}}{\mathrm{Km} + \mathrm{M}} \tag{64}$$

$$\mathrm{function\_7}\left(\mathrm{k}, \mathrm{M}, \mathrm{Km}\right) = \frac{\mathrm{k} \cdot \mathrm{M}}{\mathrm{Km} + \mathrm{M}} \tag{65}$$

9.10 Reaction reaction_10

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name v10

Notes mRNA degradation

Reaction equation

$$\mathrm{species\_8} \xrightarrow{\mathrm{species\_8}} \emptyset \tag{66}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
species_8	RNA	

Modifier

Table 30: Properties of each modifier.

Id	Name	SBO
species_8	RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{parameter\_39} \cdot \text{species\_8} \tag{67}$$

9.11 Reaction reaction_11

This is an irreversible reaction of one reactant forming one product influenced by five modifiers.

Name v7

Notes Linear phosphorylation of Hog1 by either the scaffold complex (Sho1-branch) or acti

Reaction equation

$$\text{species\_9} \xrightarrow{\text{species\_5, species\_11, species\_5, species\_9, species\_11}} \text{species\_3} \tag{68}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
species_9	Hog1P	

Modifiers

Table 32: Properties of each modifier.

Id	Name	SBO
species_5	Pbs2P	
species_11	Sho1Pbs2P	
species_5	Pbs2P	
species_9	Hog1P	
species_11	Sho1Pbs2P	

Product

Table 33: Properties of each product.

Id	Name	SBO
species_3	Hog1PP	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_3}\left(\mathrm{parameter\_25}, \frac{\mathrm{species\_5}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \frac{\mathrm{species\_9}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \mathrm{parameter\_41}, \frac{\mathrm{species\_11}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}\right) \tag{69}$$

$$\mathrm{function\_3}\left(\mathrm{k1}, \mathrm{M1}, \mathrm{S}, \mathrm{k2}, \mathrm{M2}\right) = \mathrm{k1} \cdot \mathrm{M1} \cdot \mathrm{S} + \mathrm{k2} \cdot \mathrm{M2} \cdot \mathrm{S} \tag{70}$$

$$\mathrm{function\_3}\left(\mathrm{k1}, \mathrm{M1}, \mathrm{S}, \mathrm{k2}, \mathrm{M2}\right) = \mathrm{k1} \cdot \mathrm{M1} \cdot \mathrm{S} + \mathrm{k2} \cdot \mathrm{M2} \cdot \mathrm{S} \tag{71}$$

9.12 Reaction reaction_12

This is an irreversible reaction of one reactant forming one product influenced by three modifiers.

Name v8

Notes Constitutive phosphatase dependent de-phosphorylation.

Reaction equation

$$\mathrm{species\_3} \xrightarrow{\mathrm{species\_6,\ species\_6,\ species\_3}} \mathrm{species\_9} \tag{72}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
species_3	Hog1PP	

Modifiers

Table 35: Properties of each modifier.

Id	Name	SBO
species_6	Phosphatase	
species_6	Phosphatase	
species_3	Hog1PP	

Product

Table 36: Properties of each product.

Id	Name	SBO
species_9	Hog1P	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_2}\left(\mathrm{parameter\_26}, \frac{\mathrm{species\_6}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \frac{\mathrm{species\_3}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}\right) \tag{73}$$

$$\mathrm{function\_2}\left(\mathrm{k}, \mathrm{M}, \mathrm{S}\right) = \mathrm{k} \cdot \mathrm{M} \cdot \mathrm{S} \tag{74}$$

$$\mathrm{function\_2}\left(\mathrm{k}, \mathrm{M}, \mathrm{S}\right) = \mathrm{k} \cdot \mathrm{M} \cdot \mathrm{S} \tag{75}$$

9.13 Reaction reaction_13

This is an irreversible reaction of one reactant forming two products influenced by one modifier.

Name v4

Notes Constitutive dissociation of the scaffold complex.

Reaction equation

$$\text{species\_11} \xrightarrow{\text{species\_11}} \text{species\_10} + \text{species\_4} \tag{76}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
species_11	Sho1Pbs2P	

Modifier

Table 38: Properties of each modifier.

Id	Name	SBO
species_11	Sho1Pbs2P	

Products

Table 39: Properties of each product.

Id	Name	SBO
species_10	Sho1	
species_4	Pbs2	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{parameter\_79} \cdot \text{species\_11} \tag{77}$$

9.14 Reaction reaction_14

This is an irreversible reaction of two reactants forming one product influenced by four modifiers.

Name v3_fb

Notes Simple cell surface area dependent binding of Pbs2 to Sho1. The complex is supposed

Reaction equation

$$\text{species\_4} + \text{species\_10} \xrightarrow{\text{species\_12, species\_4, species\_10, species\_12}} \text{species\_11} \tag{78}$$

Reactants

Table 40: Properties of each reactant.

Id	Name	SBO
species_4	Pbs2	
species_10	Sho1	

Modifiers

Table 41: Properties of each modifier.

Id	Name	SBO
species_12	Hog1PPActive	
species_4	Pbs2	
species_10	Sho1	
species_12	Hog1PPActive	

Product

Table 42: Properties of each product.

Id	Name	SBO
species_11	Sho1Pbs2P	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} v_{14} = {} & \text{vol}(\text{compartment\_1}) \\ & \cdot \text{function\_8}\left(\text{parameter\_57}, \text{parameter\_82}, \text{parameter\_56}, \frac{\text{species\_4}}{\text{vol}(\text{compartment\_1})}, \right. \\ & \left. \frac{\text{species\_10}}{\text{vol}(\text{compartment\_1})}, \frac{\text{species\_12}}{\text{vol}(\text{compartment\_1})}, \text{parameter\_80}, \text{parameter\_81}\right) \end{aligned} \tag{79}$$

$$\text{function\_8}(\text{ko}, \text{k}, \text{M1}, \text{S1}, \text{S2}, \text{M2}, \text{Ki}, \text{h}) = \frac{\text{ko} \cdot \text{k} \cdot \text{M1} \cdot \text{S1} \cdot \text{S2}}{1 + \left(\frac{\text{M2}}{\text{Ki}}\right)^{\text{h}}} \tag{80}$$

$$\text{function\_8}(\text{ko},\text{k},\text{M1},\text{S1},\text{S2},\text{M2},\text{Ki},\text{h}) = \frac{\text{ko}\cdot\text{k}\cdot\text{M1}\cdot\text{S1}\cdot\text{S2}}{1+\left(\frac{\text{M2}}{\text{Ki}}\right)^{\text{h}}} \tag{81}$$

9.15 Reaction `reaction_15`

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Name v15_5

Notes `Turgor dependent closure of Fps1, in conjunction with v16_5, v16_6, v16_7, v16_8.`

Reaction equation

$$\text{species\_14} \xrightarrow{\text{species\_14}} \text{species\_15} \tag{82}$$

Reactant

Table 43: Properties of each reactant.

Id	Name	SBO
`species_14`	Fps1	

Modifier

Table 44: Properties of each modifier.

Id	Name	SBO
`species_14`	Fps1	

Product

Table 45: Properties of each product.

Id	Name	SBO
`species_15`	Fps1P	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\left(\mathrm{compartment\_4}\right) \cdot \mathrm{function\_9}\left(\mathrm{parameter\_71}, \mathrm{parameter\_83}, \mathrm{parameter\_63}, \frac{\mathrm{species\_14}}{\mathrm{vol}\left(\mathrm{compartment\_4}\right)}\right) \tag{83}$$

$$\mathrm{function\_9}\left(\mathrm{ko}, \mathrm{k}, \mathrm{M}, \mathrm{S}\right) = \mathrm{ko} \cdot \mathrm{k} \cdot \mathrm{M} \cdot \mathrm{S} \tag{84}$$

$$\mathrm{function\_9}\left(\mathrm{ko}, \mathrm{k}, \mathrm{M}, \mathrm{S}\right) = \mathrm{ko} \cdot \mathrm{k} \cdot \mathrm{M} \cdot \mathrm{S} \tag{85}$$

9.16 Reaction `reaction_16`

This is an irreversible reaction of one reactant forming one product influenced by three modifiers.

Name v16_6

Notes `Activated Hog1 inhibited channel opening, in conjunction with v15_5.`

Reaction equation

$$\mathrm{species\_15} \xrightarrow{\mathrm{species\_12},\ \mathrm{species\_15},\ \mathrm{species\_12}} \mathrm{species\_14} \tag{86}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
`species_15`	Fps1P	

Modifiers

Table 47: Properties of each modifier.

Id	Name	SBO
`species_12`	Hog1PPActive	
`species_15`	Fps1P	
`species_12`	Hog1PPActive	

Product

Table 48: Properties of each product.

Id	Name	SBO
species_14	Fps1	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\left(\mathrm{compartment\_4}\right) \cdot \mathrm{function\_10}\left(\mathrm{parameter\_71}, \mathrm{parameter\_65}, \frac{\mathrm{species\_15}}{\mathrm{vol}\left(\mathrm{compartment\_4}\right)}, \frac{\mathrm{species\_12}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \mathrm{parameter\_84}, \mathrm{parameter\_85}\right) \tag{87}$$

$$\mathrm{function\_10}\left(\mathrm{ko}, \mathrm{k}, \mathrm{S}, \mathrm{M}, \mathrm{Ki}, \mathrm{h}\right) = \frac{\mathrm{ko} \cdot \mathrm{k} \cdot \mathrm{S}}{1 + \left(\frac{\mathrm{M}}{\mathrm{Ki}}\right)^{\mathrm{h}}} \tag{88}$$

$$\mathrm{function\_10}\left(\mathrm{ko}, \mathrm{k}, \mathrm{S}, \mathrm{M}, \mathrm{Ki}, \mathrm{h}\right) = \frac{\mathrm{ko} \cdot \mathrm{k} \cdot \mathrm{S}}{1 + \left(\frac{\mathrm{M}}{\mathrm{Ki}}\right)^{\mathrm{h}}} \tag{89}$$

10 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.

10.1 Species species_1

Name Glyin

Notes `Intracellular glycerol, approximated by assuming a measured value of 0.1 mM/OD in 1 18106 cells per ml sample culture and an average osmotic cell volume of 29.5 fl, i.e`

Initial amount 5310000 µmol

Initial assignment `species_1`

This species takes part in three reactions (as a reactant in reaction_8 and as a product in reaction_7 and as a modifier in reaction_8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_1} = v_7 - v_8 \tag{90}$$

10.2 Species species_2

Name Hog1

Notes MAP kinase

Initial amount 9.6760009944572 µmol

Initial assignment species_2

This species takes part in three reactions (as a reactant in reaction_3 and as a product in reaction_4 and as a modifier in reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_2} = v_4 - v_3 \tag{91}$$

10.3 Species species_3

Name Hog1PP

Notes Double phosphorylated, i.e. active, MAP kinase. It was derived from data that 2.23

Initial amount 0.201092527399535 µmol

Initial assignment species_3

This species takes part in three reactions (as a reactant in reaction_12 and as a product in reaction_11 and as a modifier in reaction_12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_3} = v_{11} - v_{12} \tag{92}$$

10.4 Species species_4

Name Pbs2

Notes MAP kinase kinase

Initial amount 3.57956846222666 µmol

Initial assignment species_4

This species takes part in six reactions (as a reactant in reaction_1, reaction_14 and as a product in reaction_2, reaction_13 and as a modifier in reaction_1, reaction_14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_4} = v_2 + v_{13} - v_1 - v_{14} \tag{93}$$

10.5 Species species_5

Name Pbs2P

Notes Activated MAP kinase kinase (Sln1 branch). Initial condition set such that a steady

Initial amount 0.00385515442085361 µmol

Initial assignment species_5

This species takes part in seven reactions (as a reactant in reaction_2 and as a product in reaction_1 and as a modifier in reaction_2, reaction_3, reaction_3, reaction_11, reaction_11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_5} = v_1 - v_2 \tag{94}$$

10.6 Species species_6

Name Phosphatase

Notes Placeholder for phosphatases like Ppt1/2/3 and others. Initial value derived from r

Initial amount 1.27698439056792 µmol

Initial assignment species_6

This species takes part in six reactions (as a modifier in reaction_2, reaction_2, reaction_4, reaction_4, reaction_12, reaction_12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_6} = 0 \tag{95}$$

10.7 Species species_7

Name Protein

Notes Placeholder for Hog1-dependent proteins, especially Gpd1. Initial value derived fro

Initial amount 1.34008635004982 µmol

Initial assignment species_7

This species takes part in five reactions (as a reactant in reaction_6 and as a product in reaction_5 and as a modifier in reaction_6, reaction_7, reaction_7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_7} = v_5 - v_6 \tag{96}$$

10.8 Species species_8

Name RNA

Notes Placeholder for transcribed genes. Initial value derived from data, i.e. initial pe

Initial amount 1.003 µmol

Initial assignment species_8

This species takes part in five reactions (as a reactant in reaction_10 and as a product in reaction_9 and as a modifier in reaction_5, reaction_5, reaction_10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_8} = v_9 - v_{10} \tag{97}$$

10.9 Species species_9

Name Hog1P

Notes Single phosphorylated MAP kinase. Initial condition set such that a steady state of

Initial amount 1.39490913506788 µmol

Initial assignment species_9

This species takes part in six reactions (as a reactant in reaction_4, reaction_11 and as a product in reaction_3, reaction_12 and as a modifier in reaction_4, reaction_11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_9} = v_3 + v_{12} - v_4 - v_{11} \tag{98}$$

10.10 Species species_10

Name Sho1

Notes One of the putative upstream sensors

Initial amount 3.86572185643496 µmol

Initial assignment species_10

This species takes part in three reactions (as a reactant in reaction_14 and as a product in reaction_13 and as a modifier in reaction_14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_10} = v_{13} - v_{14} \tag{99}$$

10.11 Species species_11

Name Sho1Pbs2P

Notes `Active scaffold complex (Sho1 branch). Initial condition set such that a steady sta`

Initial amount 0.00342460653415448 µmol

Initial assignment `species_11`

This species takes part in seven reactions (as a reactant in reaction_13 and as a product in reaction_14 and as a modifier in reaction_3, reaction_3, reaction_11, reaction_11, reaction_13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_11} = v_{14} - v_{13} \tag{100}$$

10.12 Species species_12

Name Hog1PPActive

Initial amount 0.201092527399535 µmol

Involved in rule species_12

This species takes part in ten reactions (as a modifier in reaction_1, reaction_1, reaction_7, reaction_7, reaction_9, reaction_9, reaction_14, reaction_14, reaction_16, reaction_16). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

10.13 Species species_13

Name Glyex

Notes `Extracellular glycerol, assumed to be 100 times lower than Gly_in.`

Initial amount $9 \cdot 10^7$ µmol

Initial assignment `species_13`

This species takes part in two reactions (as a product in reaction_8 and as a modifier in reaction_8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_13} = v_8 \tag{101}$$

10.14 Species species_14

Name Fps1

Notes Membrane bound open form of aquaglyceroporin Fps1 (assumed to be independent from

Initial amount 0.0255278667484759 µmol

Initial assignment species_14

This species takes part in three reactions (as a reactant in reaction_15 and as a product in reaction_16 and as a modifier in reaction_15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_14} = v_{16} - v_{15} \tag{102}$$

10.15 Species species_15

Name Fps1P

Notes Membrane bound closed form of aquaglyceroporin Fps1 (assumed to be independent fro

Initial amount 0.0255278667484759 µmol

Initial assignment species_15

This species takes part in three reactions (as a reactant in reaction_16 and as a product in reaction_15 and as a modifier in reaction_16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_15} = v_{15} - v_{16} \tag{103}$$

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