SBML Model Report

Model name: "Liu2010_Hormonal_Crosstalk_Arabidopsis"



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Lukas Endler¹ and Junli Liu² at September 20th 2010 at 5:04 p.m. and last time modified at February eighth 2012 at 7:28 p.m. Table 1 gives 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	2
species types	0	species	18
events	0	constraints	0
reactions	22	function definitions	18
global parameters	32	unit definitions	6
rules	3	initial assignments	0

Model Notes

This is the single cell model for analysis of hormonal crosstalk in Arabidopsis described in the article:

Modelling and experimental analysis of hormonal crosstalk in Arabidopsis.

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Liu J, Mehdi S, Topping J, Tarkowski P and Lindsey K. Mol Syst Biol. 2010 Jun 8;6:373; PmID: 20531403, DOI: 10.1038/msb.2010.26

Abstract:

An important question in plant biology is how genes influence the crosstalk between hormones to regulate growth. In this study, we model POLARIS (PLS) gene function and crosstalk between auxin, ethylene and cytokinin in Arabidopsis. Experimental evidence suggests that PLS acts on or close to the ethylene receptor ETR1, and a mathematical model describing possible PLS-ethylene pathway interactions is developed, and used to make quantitative predictions about PLS-hormone interactions. Modelling correctly predicts experimental results for the effect of the pls gene mutation on endogenous cytokinin concentration. Modelling also reveals a role for PLS in auxin biosynthesis in addition to a role in auxin transport. The model reproduces available mutants, and with new experimental data provides new insights into how PLS regulates auxin concentration, by controlling the relative contribution of auxin transport and biosynthesis and by integrating auxin, ethylene and cytokinin signalling. Modelling further reveals that a bell-shaped dose-response relationship between endogenous auxin and root length is established via PLS. This combined modelling and experimental analysis provides new insights into the integration of hormonal signals in plants.

This model was originally created using Copasi and taken from the supplementary materials of the MSB article. It uses equation 5 for the auxin biosynthesis and was altered to also contain the reactions for ACC, IAA and cytokinine import. Different from the supplementary material, the parameters for the auxin synthesis, v2, are set to k2c = 0.01 uM and k2=0.2 uM_per_sec and for the WT PLS transcription k6=0.3. To obtain the model described in the first table of the supplementary materials, set k2c=k2=0 and k6=0.9. For the pls and PLSox mutants, k6 should be set to 0 and 0.45, respectively.

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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 nine unit definitions of which three are predefined by SBML and not mentioned in the model.

2.1 Unit substance

Name umole

Definition µmol

2.2 Unit uM

Name uM

Definition $\mu mol \cdot l^{-1}$

2.3 Unit time

Name sec

Definition s

2.4 Unit per_s

Name per_sec

Definition s^{-1}

2.5 Unit per_uM_per_s

Name per_uM_per_sec

Definition $\mu mol^{-1} \cdot l \cdot s^{-1}$

2.6 Unit uM_per_s

Name per_uM_per_sec

Definition $\mu mol \cdot 1^{-1} \cdot s^{-1}$

2.7 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.8 Unit area

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

Definition m^2

2.9 Unit length

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

Definition m

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment_1 extra	cell extracellular	0000290	3 3	1 1	litre litre	1	

3.1 Compartment compartment_1

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

Name cell

SBO:0000290 physical compartment

3.2 Compartment extra

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

Name extracellular

4 Species

This model contains 18 species. The boundary condition of nine of these species is set to true so that these species' amount cannot be changed by any reaction. Section 9 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
		2 0 1 1 p			Condi-
					tion
Auxin	Auxin	${\tt compartment_1}$	$\mu mol \cdot l^{-1}$		
X	X	${\tt compartment_1}$	μ mol·l ⁻¹		\Box
PLSp	PLSp	${\tt compartment_1}$	μ mol·l ⁻¹		\Box
Ra	Ra	${\tt compartment_1}$	μ mol·l ⁻¹		
Ra_star	Ra*	${\tt compartment_1}$	μ mol·l ⁻¹		
RaT	Ra_total	${\tt compartment_1}$	$\mu mol \cdot l^{-1}$		
CK	CK	${\tt compartment_1}$	$\mu mol \cdot l^{-1}$		
ET	ET	${\tt compartment_1}$	$\mu mol \cdot l^{-1}$		
PLSm	PLSm	${\tt compartment_1}$	μ mol·l ⁻¹		
Re	Re	${\tt compartment_1}$	μ mol·l ⁻¹		\checkmark
ReT	Re_total	${\tt compartment_1}$	μ mol·l ⁻¹		
Re_star	Re*	${\tt compartment_1}$	μ mol·l ⁻¹		
CTR1	CTR1	${\tt compartment_1}$	$\mu mol \cdot l^{-1}$		
CTR1T	CTR1_total	${\tt compartment_1}$	μ mol·l ⁻¹		
$\mathtt{CTR1_star}$	CTR1*	${\tt compartment_1}$	$\mu mol \cdot l^{-1}$		
IAA	IAA	extra	μ mol·l ⁻¹		\square
ACC	ACC	extra	μ mol·l ⁻¹		
CK_ex	Cytokinin_ext	extra	$\mu mol \cdot l^{-1}$		\square

5 Parameters

This model contains 32 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1a	k1a	0000186	1.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	Ø
k1	k1	0000288	1.000	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
k2	k2	0000485	0.200	$\mu \text{mol} \cdot l^{-1} \cdot s^{-1}$	
k2a	k2a	0000046	2.800	s^{-1}	
k2b	k2b	0000288	1.000	μ mol·l ⁻¹	
k2c	k2c	0000027	0.010	μ mol·l ⁻¹	
k3	k3	0000035	2.000	s^{-1}	
k3a	k3a	0000036	0.450	$\mu mol^{-1} \cdot l \cdot s^{-1}$	
k4	k4	0000036	1.000	$\mu \text{mol}^{-1} \cdot l \cdot s^{-1}$	
k5	k5	0000035	1.000	s^{-1}	$\overline{\mathbf{Z}}$
k6	k6	0000035	0.300	s^{-1}	
k6a	k6a	0000288	0.200	μ mol·l ⁻¹	
k7	k7	0000035	1.000	s^{-1}	
k8	k8	0000035	1.000	s^{-1}	
k9	k9	0000035	1.000	s^{-1}	
k10	k10	0000035	$3 \cdot 10^{-4}$	s^{-1}	
k10a	k10a	0000036	0.500	$\mu \text{mol}^{-1} \cdot l \cdot s^{-1}$	
k11	k11	0000036	5.000	$\mu \text{mol}^{-1} \cdot l \cdot s^{-1}$	
k12	k12	0000035	0.100	$\mu mol \cdot l^{-1} \cdot s^{-1}$	
k12a	k12a	0000036	0.100	$\mu \text{mol}^{-1} \cdot l \cdot s^{-1}$	
k13	k13	0000035	1.000	s^{-1}	
k14	k14	0000036	3.000	$\mu \text{mol}^{-1} \cdot l \cdot s^{-1}$	
k15	k15	0000035	0.085	s^{-1}	
k16	k16	0000324	0.300	$\mu mol \cdot l^{-1} \cdot s^{-1}$	
k16a	k16a	0000038	1.000	s^{-1}	$\overline{\mathbf{Z}}$
k17	k17	0000035	0.100	s^{-1}	$\overline{\mathbf{Z}}$
k18a	k18a	0000324	1.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	$\overline{\mathbf{Z}}$
k18	k18	0000288	0.100	μ mol \cdot l ⁻¹	$\overline{\mathbf{Z}}$
k19	k19	0000035	1.000	s^{-1}	$\overline{\mathbf{Z}}$
k_{-} ethylene	k_ethylene	0000035	0.500	s^{-1}	$\overline{\mathbf{Z}}$
k_auxin	k_auxin	0000035	70.000	s^{-1}	$\overline{\mathbf{Z}}$
$k_{\tt cytokinin}$	k_cytokinin	0000035	10.000	s^{-1}	\overline{Z}

6 Function definitions

This is an overview of 18 function definitions.

6.1 Function definition function_1

Name Rate law for v3: Auxin removal from the cell

Arguments k3, k3a, [X], [Auxin]

Mathematical Expression

$$(k3 + k3a \cdot [X]) \cdot [Auxin] \tag{1}$$

6.2 Function definition function_2

Name Rate law for v1: Auxin Transport to the cell

Arguments k1a, [X], k1

Mathematical Expression

$$\frac{k1a}{1 + \frac{[X]}{k1}} \tag{2}$$

6.3 Function definition function_3

Name Rate law for v2: Auxin biosynthesis in the cell

Arguments k2, k2a, [ET], [CK], k2b, [PLSp], k2c

Mathematical Expression

$$k2 + k2a \cdot \frac{[ET]}{1 + \frac{[CK]}{k2b}} \cdot \frac{[PLSp]}{k2c + [PLSp]}$$
 (3)

6.4 Function definition function_4

Name Rate law for v4: Conversion of auxin receptor from the inactivated form to the activated form

Arguments k4, [Auxin], [Ra]

Mathematical Expression

$$k4 \cdot [Auxin] \cdot [Ra] \tag{4}$$

6.5 Function definition function_6

Name Rate law for v6: Transcription of POLARIS gene

Arguments k6, [Ra_star], [ET], k6a

Mathematical Expression

$$\frac{\text{k6} \cdot [\text{Ra_star}]}{1 + \frac{[\text{ET}]}{\text{k6a}}} \tag{5}$$

6.6 Function definition function_7

Name Rate law for v7: Decay of mRNA of POLARIS gene

Arguments k7, [PLSm]

Mathematical Expression

$$k7 \cdot [PLSm]$$
 (6)

6.7 Function definition function_8

Name Rate law for v8: Translation of POLARIS gene

Arguments k8, [PLSm]

Mathematical Expression

$$k8 \cdot [PLSm]$$
 (7)

6.8 Function definition function_9

Name Rate law for v9: Decay of protein of POLARIS gene

Arguments k9, [PLSp]

Mathematical Expression

$$k9 \cdot [PLSp]$$
 (8)

6.9 Function definition function_10

Name Rate law for v10: Conversion of the inactivated form of ethylene receptor to its activated form by PLSp

Arguments k10, [PLSp], k10a, [Re]

Mathematical Expression

$$(k10 + k10a \cdot [PLSp]) \cdot [Re] \tag{9}$$

6.10 Function definition function_12

Name Rate law for v11: Conversion of the activated form of ethylene receptor to its inactivated form

Arguments [Re_star], [ET], k11

Mathematical Expression

$$k11 \cdot [Re_star] \cdot [ET]$$
 (10)

6.11 Function definition function_13

Name Rate law for v12: Ethylene biosynthesis

Arguments [Auxin], [CK], k12, k12a

Mathematical Expression

$$k12 + k12a \cdot [Auxin] \cdot [CK] \tag{11}$$

6.12 Function definition function_15

Name Rate law for v13: Removal of ethylene

Arguments [ET], k13

Mathematical Expression

$$k13 \cdot [ET] \tag{12}$$

6.13 Function definition function_16

Name Rate law for v14: Conversion of the inactivated form of CTR1 protein to its activated form by Re*

Arguments [Re_star], k14, [CTR1]

Mathematical Expression

$$k14 \cdot [Re_star] \cdot [CTR1] \tag{13}$$

6.14 Function definition function_17

Name Rate law for v15: Conversion of the activated form of CTR1 protein to its inactivated form

Arguments [CTR1_star], k15

Mathematical Expression

$$k15 \cdot [CTR1_star]$$
 (14)

6.15 Function definition function_20

Name Rate law for v18: Biosynthesis of cytokinin

Arguments [Auxin], k18a, k18

Mathematical Expression

$$\frac{k18a}{1 + \frac{[Auxin]}{k18}}\tag{15}$$

6.16 Function definition function_18

Name Rate law for v16: Activation of the downstream of ethylene signalling response is inhibited by CTR1*

Arguments [CTR1_star], k16, k16a

Mathematical Expression

$$k16 - k16a \cdot [CTR1_star] \tag{16}$$

6.17 Function definition function_19

Name Rate law for v17: Removal of the unknown molecule X

Arguments [X], k17

Mathematical Expression

$$k17 \cdot [X] \tag{17}$$

6.18 Function definition function_21

Name Rate law for v19: removal of cytokinin

Arguments [CK], k19

Mathematical Expression

$$k19 \cdot [CK] \tag{18}$$

7 Rules

This is an overview of three rules.

7.1 Rule Ra

Rule Ra is an assignment rule for species Ra:

$$Ra = [RaT] - [Ra_star]$$
 (19)

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

7.2 Rule Re

Rule Re is an assignment rule for species Re:

$$Re = [ReT] - [Re_star]$$
 (20)

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

7.3 Rule CTR1

Rule CTR1 is an assignment rule for species CTR1:

$$CTR1 = [CTR1T] - [CTR1_star]$$
 (21)

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

12

8 Reactions

This model contains 22 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

Νō	Id	Name	Reaction Equation	SBO
1	${\tt reaction_1}$	v1: Auxin Transport to the cell	$\emptyset \xrightarrow{X} Auxin$	0000185
2	reaction_2	v2: Auxin biosynthesis in the cell	$\emptyset \xrightarrow{ET, CK, PLSp} Auxin$	0000393
3	reaction_3	v3: Auxin removal from the cell	$\operatorname{Auxin} \xrightarrow{X} \emptyset$	0000179
4	reaction_4	v4: Conversion of auxin receptor from the in- activated form to the activated form	Ra Auxin Ra_star	0000176
5	reaction_5	v5: Conversion of auxin receptor from the activated form to the inactivated form	$Ra_star \longrightarrow Ra$	0000176
6	${\tt reaction_6}$	v6: Transcription of POLARIS gene	$\emptyset \xrightarrow{\text{Ra_star, ET}} \text{PLSm}$	0000183
7	${\tt reaction_7}$	v7: Decay of mRNA of POLARIS gene	$PLSm \longrightarrow \emptyset$	0000179
8	reaction_8	v8: Translation of POLARIS gene	$\emptyset \xrightarrow{\text{PLSm}} \text{PLSp}$	0000184
9	${\tt reaction_9}$	v9: Decay of protein of POLARIS gene	$PLSp \longrightarrow \emptyset$	0000179
10	reaction_10	v10: Conversion of the inactivated form of ethylene receptor to its activated form by PLSp	$Re \xrightarrow{PLSp} Re_star$	0000176
11	reaction_11	v11: Conversion of the activated form of ethylene receptor to its inactivated form	$Re_star \xrightarrow{ET} Re$	0000176
12	reaction_12	v12: Ethylene biosynthesis	$\emptyset \xrightarrow{\text{Auxin, CK}} \text{ET}$	0000393
13	reaction_13	v13: Removal of ethylene	$ET \longrightarrow \emptyset$	0000179

N⁰	Id	Name	Reaction Equation	SBO
14	reaction_14	v14: Conversion of the inactivated form of CTR1 protein to its activated form by Re*	$CTR1 \xrightarrow{Re_star} CTR1_star$	0000176
15	reaction_15	v15: Conversion of the activated form of CTR1 protein to its inactivated form	$CTR1_star \longrightarrow CTR1$	0000176
16	reaction_16	v16: Activation of the downstream of ethylene signalling response is inhibited by CTR1*	$\emptyset \xrightarrow{CTR1_star} X$	0000176
17	reaction_17	v17: Removal of the unknown molecule X	$X \longrightarrow \emptyset$	0000179
18	reaction_18	v18: Biosynthesis of cytokinin	$\emptyset \xrightarrow{\text{Auxin}} \text{CK}$	0000393
19	reaction_19	v19: removal of cytokinin	$CK \longrightarrow \emptyset$	0000179
20	v_Ethylene	vEthylene: Uptake rate of exogenous ACC (1-aminocyclopropane-1-carboxylic acid)	$ACC \longrightarrow ET$	0000185
21	v_Auxin	vAuxin: Uptake rate of exogenous auxin (indole-3-acetic acid, IAA)	$IAA \longrightarrow Auxin$	0000185
22	$v_Cytokinin$	vCytokinin: Uptake rate of exogenous cytokinin	$CK_ex \longrightarrow CK$	0000185

8.1 Reaction reaction_1

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

Name v1: Auxin Transport to the cell

SBO:0000185 transport reaction

Reaction equation

$$\emptyset \xrightarrow{X} Auxin$$
 (22)

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
X	X	0000020

Product

Table 7: Properties of each product.

Id	Name	SBO
Auxin	Auxin	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol} \left(\text{compartment_1} \right) \cdot \text{function_2} \left(\text{k1a}, [\text{X}], \text{k1} \right)$$
 (23)

function_2
$$(k1a, [X], k1) = \frac{k1a}{1 + \frac{[X]}{k1}}$$
 (24)

function_2 (k1a, [X], k1) =
$$\frac{k1a}{1 + \frac{[X]}{k1}}$$
 (25)

8.2 Reaction reaction_2

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

Name v2: Auxin biosynthesis in the cell

SBO:0000393 production

Reaction equation

$$\emptyset \xrightarrow{\text{ET, CK, PLSp}} \text{Auxin} \tag{26}$$

Modifiers

Table 8: Properties of each modifier.

Id	Name	SBO
ET	ET	0000459
CK	CK	0000020
PLSp	PLSp	0000460

Product

Table 9: Properties of each product.

Id	Name	SBO
Auxin	Auxin	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol} \left(\text{compartment_1} \right) \cdot \text{function_3} \left(\text{k2}, \text{k2a}, [\text{ET}], [\text{CK}], \text{k2b}, [\text{PLSp}], \text{k2c} \right)$$
 (27)

$$function_3 (k2, k2a, [ET], [CK], k2b, [PLSp], k2c) = k2 + k2a \cdot \frac{[ET]}{1 + \frac{[CK]}{k2b}} \cdot \frac{[PLSp]}{k2c + [PLSp]}$$
(28)

$$function_3 \left(k2, k2a, [ET], [CK], k2b, [PLSp], k2c \right) = k2 + k2a \cdot \frac{[ET]}{1 + \frac{[CK]}{k2b}} \cdot \frac{[PLSp]}{k2c + [PLSp]} \quad (29)$$

8.3 Reaction reaction_3

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

Name v3: Auxin removal from the cell

SBO:0000179 degradation

Reaction equation

$$\operatorname{Auxin} \xrightarrow{\mathbf{X}} \emptyset \tag{30}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
Auxin	Auxin	

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
X	X	0000459

Kinetic Law

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

$$v_3 = \text{vol} \left(\text{compartment_1} \right) \cdot \text{function_1} \left(\text{k3}, \text{k3a}, [\text{X}], [\text{Auxin}] \right)$$
 (31)

$$function_1(k3, k3a, [X], [Auxin]) = (k3 + k3a \cdot [X]) \cdot [Auxin]$$
(32)

$$function_1(k3, k3a, [X], [Auxin]) = (k3 + k3a \cdot [X]) \cdot [Auxin]$$
(33)

8.4 Reaction reaction_4

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

Name v4: Conversion of auxin receptor from the inactivated form to the activated form

SBO:0000176 biochemical reaction

Reaction equation

$$Ra \xrightarrow{Auxin} Ra_star$$
 (34)

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Ra	Ra	

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
Auxin	Auxin	0000461

Product

Table 14: Properties of each product.

Id	Name	SBO
Ra_star	Ra*	

Kinetic Law

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

$$v_4 = \text{vol}\left(\text{compartment}_1\right) \cdot \text{function}_4\left(\text{k4}, [\text{Auxin}], [\text{Ra}]\right)$$
 (35)

$$function_4(k4, [Auxin], [Ra]) = k4 \cdot [Auxin] \cdot [Ra]$$
(36)

$$function_4(k4, [Auxin], [Ra]) = k4 \cdot [Auxin] \cdot [Ra]$$
(37)

8.5 Reaction reaction_5

This is an irreversible reaction of one reactant forming one product.

Name v5: Conversion of auxin receptor from the activated form to the inactivated form

SBO:0000176 biochemical reaction

Reaction equation

$$Ra_star \longrightarrow Ra \tag{38}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
Ra_star	Ra*	

Product

Table 16: Properties of each product.

Id	Name	SBO
Ra	Ra	

Kinetic Law

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

$$v_5 = \text{vol} \left(\text{compartment}_{-1} \right) \cdot \text{k5} \cdot \left[\text{Ra_star} \right]$$
 (39)

8.6 Reaction reaction_6

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

Name v6: Transcription of POLARIS gene

SBO:0000183 transcription

Reaction equation

$$\emptyset \xrightarrow{\text{Ra_star, ET}} \text{PLSm} \tag{40}$$

Modifiers

Table 17: Properties of each modifier.

Id	Name	SBO
Ra_star	Ra*	0000461
ET	ET	0000020

Product

Table 18: Properties of each product.

Id	Name	SBO
PLSm	PLSm	

Derived unit contains undeclared units

$$v_6 = \text{vol}\left(\text{compartment_1}\right) \cdot \text{function_6}\left(\text{k6}, [\text{Ra_star}], [\text{ET}], \text{k6a}\right)$$
 (41)

$$function_6\left(k6,[Ra_star],[ET],k6a\right) = \frac{k6\cdot[Ra_star]}{1+\frac{[ET]}{k6a}} \tag{42}$$

$$function_6\left(k6,[Ra_star],[ET],k6a\right) = \frac{k6\cdot[Ra_star]}{1+\frac{[ET]}{k6a}} \tag{43}$$

8.7 Reaction reaction_7

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

Name v7: Decay of mRNA of POLARIS gene

SBO:0000179 degradation

Reaction equation

$$PLSm \longrightarrow \emptyset \tag{44}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
PLSm	PLSm	

Kinetic Law

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

$$v_7 = \text{vol} \left(\text{compartment_1} \right) \cdot \text{function_7} \left(\text{k7}, [\text{PLSm}] \right)$$
 (45)

$$function_{-}7 (k7, [PLSm]) = k7 \cdot [PLSm]$$
(46)

8.8 Reaction reaction_8

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

Name v8: Translation of POLARIS gene

SBO:0000184 translation

Reaction equation

$$\emptyset \xrightarrow{\text{PLSm}} \text{PLSp} \tag{48}$$

Modifier

Table 20: Properties of each modifier.

Id	Name	SBO
PLSm	PLSm	0000461

Product

Table 21: Properties of each product.

Id	Name	SBO
PLSp	PLSp	

Kinetic Law

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

$$v_8 = \text{vol}(\text{compartment_1}) \cdot \text{function_8}(\text{k8}, [\text{PLSm}])$$
 (49)

function_8 (k8, [PLSm]) =
$$k8 \cdot [PLSm]$$
 (50)

$$function_8 (k8, [PLSm]) = k8 \cdot [PLSm]$$
 (51)

8.9 Reaction reaction_9

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

Name v9: Decay of protein of POLARIS gene

SBO:0000179 degradation

Reaction equation

$$PLSp \longrightarrow \emptyset \tag{52}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
PLSp	PLSp	

Kinetic Law

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

$$v_9 = \text{vol} (\text{compartment_1}) \cdot \text{function_9} (k9, [PLSp])$$
 (53)

8.10 Reaction reaction_10

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

Name v10: Conversion of the inactivated form of ethylene receptor to its activated form by PLSp

SBO:0000176 biochemical reaction

Reaction equation

$$Re \xrightarrow{PLSp} Re_star \tag{56}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
Re	Re	

Modifier

Table 24: Properties of each modifier.

Id	Name	SBO
PLSp	PLSp	0000462

Product

Table 25: Properties of each product.

Id	Name	SBO
Re_star	Re*	

Kinetic Law

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

$$v_{10} = \text{vol}(\text{compartment_1}) \cdot \text{function_10}(\text{k10},[\text{PLSp}],\text{k10a},[\text{Re}])$$
 (57)

8.11 Reaction reaction_11

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

Name v11: Conversion of the activated form of ethylene receptor to its inactivated form

SBO:0000176 biochemical reaction

Reaction equation

$$Re_star \xrightarrow{ET} Re \tag{60}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
Re_star	Re*	

Modifier

Table 27: Properties of each modifier.

Id	Name	SBO
ET	ET	0000461

Product

Table 28: Properties of each product.

Id	Name	SBO
Re	Re	

Kinetic Law

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

$$v_{11} = \text{vol}\left(\text{compartment}_{-1}\right) \cdot \text{function}_{-12}\left([\text{Re_star}], [\text{ET}], \text{k11}\right)$$
 (61)

$$function_12([Re_star], [ET], k11) = k11 \cdot [Re_star] \cdot [ET]$$
(62)

$$function_{12}([Re_star], [ET], k11) = k11 \cdot [Re_star] \cdot [ET]$$
(63)

8.12 Reaction reaction_12

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

Name v12: Ethylene biosynthesis

SBO:0000393 production

Reaction equation

$$\emptyset \xrightarrow{\text{Auxin, CK}} \text{ET} \tag{64}$$

Modifiers

Table 29: Properties of each modifier.

Id	Name	SBO
Auxin	Auxin	0000462
CK	CK	0000462

Product

Table 30: Properties of each product.

Id	Name	SBO
ET	ET	

Kinetic Law

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

$$v_{12} = \text{vol} \left(\text{compartment}_{-1}\right) \cdot \text{function}_{-13} \left([\text{Auxin}], [\text{CK}], \text{k12}, \text{k12a}\right)$$
 (65)

function_13 ([Auxin], [CK], k12, k12a) =
$$k12 + k12a \cdot [Auxin] \cdot [CK]$$
 (66)

function_13 ([Auxin], [CK], k12, k12a) =
$$k12 + k12a \cdot [Auxin] \cdot [CK]$$
 (67)

8.13 Reaction reaction_13

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

Name v13: Removal of ethylene

SBO:0000179 degradation

Reaction equation

$$ET \longrightarrow \emptyset \tag{68}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
ET	ET	

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

$$v_{13} = \text{vol} \left(\text{compartment}_{-1} \right) \cdot \text{function}_{-15} \left([\text{ET}], \text{k13} \right)$$
 (69)

$$function_{-}15([ET], k13) = k13 \cdot [ET]$$

$$(71)$$

8.14 Reaction reaction_14

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

Name v14: Conversion of the inactivated form of CTR1 protein to its activated form by Re*

SBO:0000176 biochemical reaction

Reaction equation

$$CTR1 \xrightarrow{Re_star} CTR1_star$$
 (72)

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
CTR1	CTR1	

Modifier

Table 33: Properties of each modifier.

Id	Name	SBO
Re_star	Re*	0000460

Product

Table 34: Properties of each product.

Id	Name	SBO
CTR1_star	CTR1*	

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

$$v_{14} = \text{vol}\left(\text{compartment}_{-1}\right) \cdot \text{function}_{-16}\left([\text{Re_star}], \text{k14}, [\text{CTR1}]\right)$$
 (73)

$$function_16\left([Re_star],k14,[CTR1]\right) = k14 \cdot [Re_star] \cdot [CTR1] \tag{74}$$

$$function_16([Re_star], k14, [CTR1]) = k14 \cdot [Re_star] \cdot [CTR1]$$
(75)

8.15 Reaction reaction_15

This is an irreversible reaction of one reactant forming one product.

Name v15: Conversion of the activated form of CTR1 protein to its inactivated form

SBO:0000176 biochemical reaction

Reaction equation

$$CTR1_star \longrightarrow CTR1$$
 (76)

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
CTR1_star	CTR1*	

Product

Table 36: Properties of each product.

Id	Name	SBO
CTR1	CTR1	

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

$$v_{15} = \text{vol}(\text{compartment}_{-1}) \cdot \text{function}_{-17}([\text{CTR1_star}], \text{k15})$$
 (77)

$$function_{17}([CTR1_star], k15) = k15 \cdot [CTR1_star]$$
(78)

$$function_{17}([CTR1_star], k15) = k15 \cdot [CTR1_star]$$
(79)

8.16 Reaction reaction_16

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

Name v16: Activation of the downstream of ethylene signalling response is inhibited by CTR1*

SBO:0000176 biochemical reaction

Reaction equation

$$\emptyset \xrightarrow{\text{CTR1_star}} X \tag{80}$$

Modifier

Table 37: Properties of each modifier.

Id	Name	SBO
CTR1_star	CTR1*	0000020

Product

Table 38: Properties of each product.

Id	Name	SBO
Х	X	

Kinetic Law

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

$$v_{16} = \text{vol}(\text{compartment_1}) \cdot \text{function_18}([\text{CTR1_star}], \text{k16}, \text{k16a})$$
 (81)

function_18 ([CTR1_star], k16, k16a) =
$$k16 - k16a \cdot [CTR1_star]$$
 (82)

function_18 ([CTR1_star], k16, k16a) =
$$k16 - k16a \cdot [CTR1_star]$$
 (83)

8.17 Reaction reaction_17

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

Name v17: Removal of the unknown molecule X

SBO:0000179 degradation

Reaction equation

$$X \longrightarrow \emptyset$$
 (84)

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
X	X	

Kinetic Law

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

$$v_{17} = \text{vol}\left(\text{compartment_1}\right) \cdot \text{function_19}\left([X], \text{k17}\right)$$
 (85)

8.18 Reaction reaction_18

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

Name v18: Biosynthesis of cytokinin

SBO:0000393 production

Reaction equation

$$\emptyset \xrightarrow{\text{Auxin}} \text{CK} \tag{88}$$

Modifier

Table 40: Properties of each modifier.

Id	Name	SBO
Auxin	Auxin	0000020

Product

Table 41: Properties of each product.

Id	Name	SBO
CK	CK	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol}(\text{compartment_1}) \cdot \text{function_20}([\text{Auxin}], \text{k18a}, \text{k18})$$
 (89)

function_20 ([Auxin], k18a, k18) =
$$\frac{k18a}{1 + \frac{[Auxin]}{k18}}$$
 (90)

function_20([Auxin], k18a, k18) =
$$\frac{k18a}{1 + \frac{[Auxin]}{k18}}$$
 (91)

8.19 Reaction reaction_19

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

Name v19: removal of cytokinin

SBO:0000179 degradation

Reaction equation

$$CK \longrightarrow \emptyset$$
 (92)

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
CK	CK	

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

$$v_{19} = \text{vol}\left(\text{compartment_1}\right) \cdot \text{function_21}\left([\text{CK}], \text{k19}\right)$$
 (93)

8.20 Reaction v_Ethylene

This is an irreversible reaction of one reactant forming one product.

Name vEthylene: Uptake rate of exogenous ACC (1-aminocyclopropane-1-carboxylic acid)

SBO:0000185 transport reaction

Reaction equation

$$ACC \longrightarrow ET$$
 (96)

Reactant

Table 43: Properties of each reactant.

Id	Name	SBO
ACC	ACC	

Product

Table 44: Properties of each product.

Id	Name	SBO
ET	ET	

Kinetic Law

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

$$v_{20} = \text{vol}(\text{compartment}_1) \cdot \text{k_ethylene} \cdot [\text{ACC}]$$
 (97)

8.21 Reaction v_Auxin

This is an irreversible reaction of one reactant forming one product.

Name vAuxin: Uptake rate of exogenous auxin (indole-3-acetic acid, IAA)

SBO:0000185 transport reaction

Reaction equation

$$IAA \longrightarrow Auxin \tag{98}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
IAA	IAA	

Product

Table 46: Properties of each product.

Id	Name	SBO
Auxin	Auxin	

Kinetic Law

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

$$v_{21} = \text{vol}(\text{compartment}_1) \cdot \text{k}_{\text{a}} \text{uxin} \cdot [\text{IAA}]$$
 (99)

8.22 Reaction v_Cytokinin

This is an irreversible reaction of one reactant forming one product.

Name vCytokinin: Uptake rate of exogenous cytokinin

SBO:0000185 transport reaction

Reaction equation

$$CK_ex \longrightarrow CK$$
 (100)

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
CK_ex	Cytokinin_ext	

Product

Table 48: Properties of each product.

Id	Name	SBO
CK	CK	

Kinetic Law

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

$$v_{22} = \text{vol}(\text{compartment_1}) \cdot \text{k_cytokinin} \cdot [\text{CK_ex}]$$
 (101)

9 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.

9.1 Species Auxin

Name Auxin

SBO:0000247 simple chemical

Initial concentration $0.1 \ \mu mol \cdot l^{-1}$

This species takes part in seven reactions (as a reactant in reaction_3 and as a product in reaction_1, reaction_2, v_Auxin and as a modifier in reaction_4, reaction_12, reaction_18).

$$\frac{d}{dt}Auxin = v_1 + v_2 + v_{21} - v_3 \tag{102}$$

9.2 Species X

Name X

SBO:0000240 material entity

Initial concentration $0.1 \ \mu mol \cdot l^{-1}$

This species takes part in four reactions (as a reactant in reaction_17 and as a product in reaction_16 and as a modifier in reaction_1, reaction_3).

$$\frac{d}{dt}X = v_{16} - v_{17} \tag{103}$$

9.3 Species PLSp

Name PLSp

SBO:0000252 polypeptide chain

Initial concentration $0.1 \ \mu mol \cdot l^{-1}$

This species takes part in four reactions (as a reactant in reaction_9 and as a product in reaction_8 and as a modifier in reaction_2, reaction_10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PLSp} = v_8 - v_9 \tag{104}$$

9.4 Species Ra

Name Ra

SBO:0000297 protein complex

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

Involved in rule Ra

This species takes part in two reactions (as a reactant in reaction_4 and as a product in reaction_5). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.5 Species Ra_star

Name Ra*

SBO:0000297 protein complex

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

This species takes part in three reactions (as a reactant in reaction_5 and as a product in reaction_4 and as a modifier in reaction_6).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Ra_star} = v_4 - v_5 \tag{105}$$

9.6 Species RaT

Name Ra_total

SBO:0000297 protein complex

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{RaT} = 0\tag{106}$$

9.7 Species CK

Name CK

SBO:0000247 simple chemical

Initial concentration $0.1 \, \mu mol \cdot l^{-1}$

This species takes part in five reactions (as a reactant in reaction_19 and as a product in reaction_18, v_Cytokinin and as a modifier in reaction_2, reaction_12).

$$\frac{\mathrm{d}}{\mathrm{d}t}CK = v_{18} + v_{22} - v_{19} \tag{107}$$

9.8 Species ET

Name ET

SBO:0000247 simple chemical

Initial concentration $0.1 \ \mu mol \cdot l^{-1}$

This species takes part in six reactions (as a reactant in reaction_13 and as a product in reaction_12, v_Ethylene and as a modifier in reaction_2, reaction_6, reaction_11).

$$\frac{\mathrm{d}}{\mathrm{d}t}ET = v_{12} + v_{20} - v_{13} \tag{108}$$

9.9 Species PLSm

Name PLSm

SBO:0000278 messenger RNA

Initial concentration $0.1 \ \mu mol \cdot l^{-1}$

This species takes part in three reactions (as a reactant in reaction_7 and as a product in reaction_6 and as a modifier in reaction_8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PLSm} = v_6 - v_7 \tag{109}$$

9.10 Species Re

Name Re

SBO:0000252 polypeptide chain

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

Involved in rule Re

This species takes part in two reactions (as a reactant in reaction_10 and as a product in reaction_11). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.11 Species ReT

Name Re_total

SBO:0000252 polypeptide chain

Initial concentration $0.3 \ \mu mol \cdot l^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ReT} = 0\tag{110}$$

9.12 Species Re_star

Name Re*

SBO:0000252 polypeptide chain

Initial concentration $0.3 \, \mu \text{mol} \cdot l^{-1}$

This species takes part in three reactions (as a reactant in reaction_11 and as a product in reaction_10 and as a modifier in reaction_14).

$$\frac{d}{dt} \text{Re_star} = v_{10} - v_{11} \tag{111}$$

9.13 Species CTR1

Name CTR1

SBO:0000252 polypeptide chain

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

Involved in rule CTR1

This species takes part in two reactions (as a reactant in reaction_14 and as a product in reaction_15). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.14 Species CTR1T

Name CTR1_total

SBO:0000252 polypeptide chain

Initial concentration $0.3 \, \mu \text{mol} \cdot l^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CTR}1\mathrm{T} = 0\tag{112}$$

9.15 Species CTR1_star

Name CTR1*

SBO:0000252 polypeptide chain

Initial concentration $0.3 \, \mu \text{mol} \cdot l^{-1}$

This species takes part in three reactions (as a reactant in reaction_15 and as a product in reaction_14 and as a modifier in reaction_16).

$$\frac{d}{dt}CTR1_star = v_{14} - v_{15}$$
 (113)

9.16 Species IAA

Name IAA

SBO:0000247 simple chemical

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

This species takes part in one reaction (as a reactant in v_Auxin), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IAA} = 0\tag{114}$$

9.17 Species ACC

Name ACC

SBO:0000247 simple chemical

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

This species takes part in one reaction (as a reactant in v_Ethylene), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}ACC = 0\tag{115}$$

9.18 Species CK_ex

Name Cytokinin_ext

SBO:0000247 simple chemical

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

This species takes part in one reaction (as a reactant in v_Cytokinin), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}\mathrm{K}_{-}\mathrm{ex} = 0 \tag{116}$$

A Glossary of Systems Biology Ontology Terms

- **SBO:0000020 inhibitor:** Substance that decreases the probability of a chemical reaction without itself being consumed or transformed by the reaction
- **SBO:0000027** Michaelis constant: Substrate concentration at which the velocity of reaction is half its maximum. Michaelis constant is an experimental parameter. According to the underlying molecular mechanism it can be interpreted differently in terms of microscopic constants
- **SBO:0000035 forward unimolecular rate constant, continuous case:** Numerical parameter that quantifies the forward velocity of a chemical reaction involving only one reactant. This parameter encompasses all the contributions to the velocity except the quantity of the reactant. It is to be used in a reaction modelled using a continuous framework
- **SBO:0000036 forward bimolecular rate constant, continuous case:** Numerical parameter that quantifies the forward velocity of a chemical reaction involving two reactants. This parameter encompasses all the contributions to the velocity except the quantity of the reactants. It is to be used in a reaction modelled using a continuous framework
- **SBO:0000038** reverse unimolecular rate constant, continuous case: Numerical parameter that quantifies the reverse velocity of a chemical reaction involving only one product. This parameter encompasses all the contributions to the velocity except the quantity of the product. It is to be used in a reaction modelled using a continuous framework
- **SBO:0000046 zeroth order rate constant:** Numerical parameter that quantifies the velocity of a chemical reaction independent of the reactant quantities. This parameter encompasses all the contributions to the velocity
- **SBO:0000176 biochemical reaction:** An event involving one or more chemical entities that modifies the electrochemical structure of at least one of the participants.
- **SBO:0000179 degradation:** Complete disappearance of a physical entity

- **SBO:0000183 transcription:** Process through which a DNA sequence is copied to produce a complementary RNA
- **SBO:0000184 translation:** Process in which a polypeptide chain is produced from a messenger RNA
- **SBO:0000185 transport reaction:** Movement of a physical entity without modification of the structure of the entity
- **SBO:0000186** maximal velocity: Limiting maximal velocity of an enzymatic reaction, reached when the substrate is in large excess and all the enzyme is complexed.
- **SBO:0000240** material entity: A real thing that is defined by its physico-chemical structure.
- SBO:0000247 simple chemical: Simple, non-repetitive 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:0000278 messenger RNA:** A messenger RNA is a ribonucleic acid synthesized during the transcription of a gene, and that carries the information to encode one or several proteins
- **SBO:0000288 IC50:** Also called half maximal inhibitory concentration, it represents the concentration of an inhibitor substance that is required to suppress 50% of an effect.
- **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:0000297 protein complex:** Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608
- **SBO:0000324 forward maximal velocity:** Limiting maximal velocity of the forward reaction of a reversible enzyme, reached when the substrate is in large excess and all the enzyme is complexed.
- **SBO:0000393** production: Generation of a material or conceptual entity.
- **SBO:0000459 stimulator:** Substance that accelerates the velocity of a chemical reaction without itself being consumed or transformed.
- **SBO:0000460 enzymatic catalyst:** A substance that accelerates the velocity of a chemical reaction without itself being consumed or transformed, by lowering the free energy of the transition state. The substance acting as a catalyst is an enzyme
- **SBO:0000461 essential activator:** A substance that is absolutely required for occurrence and stimulation of a reaction

- **SBO:0000462 non-essential activator:** An activator which is not necessary for an enzymatic reaction, but whose presence will further increase enzymatic activity.
- **SBO:0000485** basal rate constant: The minimal velocity observed under defined conditions, which may or may not include the presence of an effector. For example in an inhibitory system, this would be the residual velocity observed under full inhibition. In non-essential activation, this would be the velocity in the absence of any activator

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