SBML Model Report

Model name: "Band2012_Dll-Venus_FullModel"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Leah Band[2] at April fifth 2012 at 2:38 p. m. and last time modified at April second 2014 at 0:25 a. 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	1
species types	0	species	5
events	0	constraints	0
reactions	9	function definitions	0
global parameters	10	unit definitions	0
rules	0	initial assignments	0

Model Notes

This model is from the article:
Root gravitropism is regulated by a transient lateral auxin gradient controlled by a tipping-point mechanism.

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Band LR, Wells DM, Larrieu A, Sun J, Middleton AM, French AP, Brunoud G, Sato EM, Wilson MH, Pret B, Oliva M, Swarup R, Sairanen I, Parry G, Ljung K, Beeckman T, Garibaldi JM, Estelle M, Owen MR, Vissenberg K, Hodgman TC, Pridmore TP, King JR, Vernoux T, Bennett MJ. Proc Natl Acad Sci U S A.2012 Mar 20;109(12):4668-73 22393022,

Abstract:
Gravity profoundly influences plant growth and development. Plants respond to changes in orientation by using gravitropic responses to modify their growth. Cholodny and Went hypothesized over 80 years ago that plants bend in response to a gravity stimulus by generating a lateral gradient of a growth regulator at an organ's apex, later found to be auxin. Auxin regulates root growth by targeting Aux/IAA repressor proteins for degradation. We used an Aux/IAA-based reporter, domain II (DII)-VENUS, in conjunction with a mathematical model to quantify auxin redistribution following a gravity stimulus. Our multidisciplinary approach revealed that auxin is rapidly redistributed to the lower side of the root within minutes of a 90 gravity stimulus. Unexpectedly, auxin asymmetry was rapidly lost as bending root tips reached an angle of 40 to the horizontal. We hypothesize roots use a „tipping point„ mechanism that operates to reverse the asymmetric auxin flow at the midpoint of root bending. These mechanistic insights illustrate the scientific value of developing quantitative reporters such as DII-VENUS in conjunction with parameterized mathematical models to provide high-resolution kinetics of hormone redistribution.

This model corresponds to the full model described in the article.

2 Unit Definitions

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

2.1 Unit `substance`

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

Definition mol

2.2 Unit `volume`

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.3 Unit `area`

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

Definition m^2

2.4 Unit `length`

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

Definition m

2.5 Unit `time`

Notes Second is the predefined SBML unit for `time`.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

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

3.1 Compartment `cell`

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

SBO:0000290 physical compartment

4 Species

This model contains five species. Section 7 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
auxin		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
TIR1		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
auxinTIR1		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
auxinTIR1VENUS		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
VENUS		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains ten global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kd			0.334		☑
ka			$8.22 \cdot 10^{-4}$		☑
mu			0.790		☑
ld			4.490		☑
lm			0.175		☑
la			1.150		☑
delta			0.486		☑
lambda			0.003		☑
TIR1T			18.500		☑
alpha_tr			30.500		☑

6 Reactions

This model contains nine 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	auxin-_TIR1association		auxin + TIR1 ⟶ auxinTIR1	0000526
2	auxin-_TIR1dissociation		auxinTIR1 ⟶ auxin + TIR1	0000180
3	auxin_TIR1-_VENUSassociation		auxinTIR1 + VENUS ⟶ auxinTIR1VENUS	0000526
4	auxin_TIR1-_VENUSdissociation		auxinTIR1VENUS ⟶ auxinTIR1 + VENUS	0000180
5	auxin_TIR1-_VENUSdissociationleadingtoubiquitination		auxinTIR1VENUS ⟶ auxinTIR1	0000180
6	auxinproduction		∅ ⟶ auxin	0000393
7	auxindecay		auxin ⟶ ∅	0000179
8	VENUSproduction		∅ ⟶ VENUS	0000393
9	VENUSphotobleachingdecay		VENUS ⟶ ∅	0000179

6.1 Reaction auxin_TIR1association

This is an irreversible reaction of two reactants forming one product.

SBO:0000526 protein complex formation

Reaction equation

$$\text{auxin} + \text{TIR1} \longrightarrow \text{auxinTIR1} \tag{1}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
auxin		
TIR1		

Product

Table 7: Properties of each product.

Id	Name	SBO
auxinTIR1		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{ka} \cdot [\text{auxin}] \cdot [\text{TIR1}] \tag{2}$$

6.2 Reaction auxin_TIR1dissociation

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

SBO:0000180 dissociation

Reaction equation

$$\text{auxinTIR1} \longrightarrow \text{auxin} + \text{TIR1} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
auxinTIR1		

Products

Table 9: Properties of each product.

Id	Name	SBO
auxin		
TIR1		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{kd} \cdot [\mathrm{auxinTIR1}] \tag{4}$$

6.3 Reaction auxin_TIR1_VENUSassociation

This is an irreversible reaction of two reactants forming one product.

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{auxinTIR1} + \mathrm{VENUS} \longrightarrow \mathrm{auxinTIR1VENUS} \tag{5}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
auxinTIR1		
VENUS		

Product

Table 11: Properties of each product.

Id	Name	SBO
auxinTIR1VENUS		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{la} \cdot [\mathrm{auxinTIR1}] \cdot [\mathrm{VENUS}] \tag{6}$$

6.4 Reaction auxin_TIR1_VENUSdissociation

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

SBO:0000180 dissociation

Reaction equation

$$\mathrm{auxinTIR1VENUS} \longrightarrow \mathrm{auxinTIR1} + \mathrm{VENUS} \tag{7}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
auxinTIR1VENUS		

Products

Table 13: Properties of each product.

Id	Name	SBO
auxinTIR1		
VENUS		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{ld} \cdot [\mathrm{auxinTIR1VENUS}] \tag{8}$$

6.5 Reaction auxin_TIR1_VENUSdissociationleadingtoubiquitination

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

SBO:0000180 dissociation

Reaction equation

$$\text{auxinTIR1VENUS} \longrightarrow \text{auxinTIR1} \tag{9}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
auxinTIR1VENUS		

Product

Table 15: Properties of each product.

Id	Name	SBO
auxinTIR1		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{lm} \cdot [\text{auxinTIR1VENUS}] \tag{10}$$

6.6 Reaction auxinproduction

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

SBO:0000393 production

Reaction equation

$$\emptyset \longrightarrow \text{auxin} \tag{11}$$

Product

Table 16: Properties of each product.

Id	Name	SBO
auxin		

Kinetic Law

Derived unit not available

$$v_6 = \text{alpha\_tr} \tag{12}$$

6.7 Reaction auxindecay

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

SBO:0000179 degradation

Reaction equation

$$\text{auxin} \longrightarrow \emptyset \tag{13}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
auxin		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{mu} \cdot [\text{auxin}] \tag{14}$$

6.8 Reaction VENUSproduction

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

SBO:0000393 production

Reaction equation

$$\emptyset \longrightarrow \text{VENUS} \tag{15}$$

Product

Table 18: Properties of each product.

Id	Name	SBO
VENUS		

Kinetic Law

Derived unit not available

$$v_8 = \text{delta} \tag{16}$$

6.9 Reaction VENUSphotobleachingdecay

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

SBO:0000179 degradation

Reaction equation

$$\text{VENUS} \longrightarrow \emptyset \tag{17}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
VENUS		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{lambda} \cdot [\text{VENUS}] \tag{18}$$

7 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.

7.1 Species `auxin`

SBO:0000252 polypeptide chain

Initial concentration $7.38\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in `auxin_TIR1association`, `auxindecay` and as a product in `auxin_TIR1dissociation`, `auxinproduction`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{auxin} = v_2 + v_6 - v_1 - v_7 \tag{19}$$

7.2 Species `TIR1`

SBO:0000252 polypeptide chain

Initial concentration $15.4\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in `auxin_TIR1association` and as a product in `auxin_TIR1dissociation`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TIR1} = v_2 - v_1 \tag{20}$$

7.3 Species `auxinTIR1`

SBO:0000297 protein complex

Initial concentration $0.28\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in `auxin_TIR1dissociation`, `auxin_TIR1_VENUSassociation` and as a product in `auxin_TIR1association`, `auxin_TIR1_VENUSdissociation`, `auxin_TIR1_VENUSdissociationleadingtoubiquitination`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{auxinTIR1} = v_1 + v_4 + v_5 - v_2 - v_3 \tag{21}$$

7.4 Species `auxinTIR1VENUS`

SBO:0000297 protein complex

Initial concentration $2.78\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in `auxin_TIR1_VENUSdissociation`, `auxin_TIR1_VENUSdissociationleadingtoubiquitination` and as a product in `auxin_TIR1_VENUSassociation`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{auxinTIR1VENUS} = v_3 - v_4 - v_5 \tag{22}$$

7.5 Species VENUS

SBO:0000297 protein complex

Initial concentration $40.4\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in auxin_TIR1_VENUSassociation, VENUSphotobleachingdecay and as a product in auxin_TIR1_VENUSdissociation, VENUSproduction).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{VENUS} = v_4 + v_8 - v_3 - v_9 \tag{23}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000179 degradation: Complete disappearance of a physical entity

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

SBO:0000252 polypeptide chain: Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

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

SBO:0000297 protein complex: Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608

SBO:0000393 production: Generation of a material or conceptual entity.

SBO:0000526 protein complex formation: The process by which two or more proteins interact non-covalently to form a protein complex (SBO:0000297)

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

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