SBML Model Report

Model name: "Vernoux2011_AuxinSignaling-_AuxinSingleStepInput"

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1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Vijayalakshmi Chelliah[1], Farcot Etienne[2] and Teva Vernoux[3] at April first 2011 at 10:17 a. m. and last time modified at August 23rd 2011 at 2:13 p. m. Table 1 shows an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	6
events	0	constraints	0
reactions	12	function definitions	0
global parameters	23	unit definitions	0
rules	4	initial assignments	0

Model Notes

This model is from the article:
The auxin signalling network translates dynamic input into robust patterning at the shoot apex.

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Vernoux T, Brunoud G, Farcot E, Morin V, Van den Daele H, Legrand J, Oliva M, Das P, Larrieu A, Wells D, Gudon Y, Armitage L, Picard F, Guyomarc'h S, Cellier C, Parry G, Koumproglou R, Doonan JH, Estelle M, Godin C, Kepinski S, Bennett M, De Veylder L, Traas J. Mol Syst Biol. 2011 Jul 5;7:508. 21734647 ,

Abstract:
The plant hormone auxin is thought to provide positional information for patterning during development. It is still unclear, however, precisely how auxin is distributed across tissues and how the hormone is sensed in space and time. The control of gene expression in response to auxin involves a complex network of over 50 potentially interacting transcriptional activators and repressors, the auxin response factors (ARFs) and Aux/IAAs. Here, we perform a large-scale analysis of the Aux/IAA-ARF pathway in the shoot apex of Arabidopsis, where dynamic auxin-based patterning controls organogenesis. A comprehensive expression map and full interactome uncovered an unexpectedly simple distribution and structure of this pathway in the shoot apex. A mathematical model of the Aux/IAA-ARF network predicted a strong bufferingcapacity along with spatial differences in auxin sensitivity. We then tested and confirmed these predictions using a novel auxin signalling sensor that reports input into the signalling pathway, in conjunction with the published DR5 transcriptional output reporter. Our results provide evidence that the auxin signalling network is essential to create robust patterns at the shoot apex.

Note:

Figure 3 of the supplementary material of the reference article has been reproduced here. Time evolution of all the variables in the model are plotted, under the influence of a step input of auxin level (auxin=5, when time>1000; 0.11, otherwise). pi_A is varied between 0 and 2 by steps of 0.1.

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
compartment_0000001	c_1	0000290	3	1	litre	☑	

3.1 Compartment compartment_0000001

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

Name c_1

SBO:0000290 physical compartment

4 Species

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

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
I	Aux/IAA	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
A	ARF	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
D_II	Aux/IAA:Aux/IAA	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
D_IA	Aux/IAA:ARF	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
R	mRNA	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
aux	auxin	compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 23 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
pi_I	pi_I	0000153	1.000		☑
d_r	d_r	0000356	0.007		☑
d_A	d_A	0000356	0.003		☑
d_II	d_II	0000356	0.003		☑
d_IA	d_IA	0000356	0.003		☑
k_II	k_II	0000341	1.000		☑
k_IA	k_IA	0000341	1.000		☑
B_d	B_d	0000282	100.000		☑
f_A	f_A	0000009	10.000		☑
gamma_I	gamma_I	0000009	10.000		☑
K_aux	K_aux	0000282	1.000		☑
K_II	K_II	0000282	10.000		☑
K_IA	K_IA	0000282	10.000		☑
f_c	f_c	0000009	10.000		☑
w_A	w_A	0000481	10.000		☑
w_I	w_I	0000481	10.000		☑
w_D	w_D	0000481	10.000		☑
d_I	d_I	0000356	0.050		☑
pi_A	pi_A	0000153	1.000		☑
k_Am	k_Am	0000009	10.000		☑
kprime_IA	kprime_IA	0000338	10.000		☐
kprime_II	kprime_II	0000338	10.000		☐
aux_basal	aux_basal	0000009	0.110		☐

6 Rules

This is an overview of four rules.

6.1 Rule aux

Rule aux is an assignment rule for species aux:

$$\text{aux} = \begin{cases} 5 & \text{if time} > 1000 \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

6.2 Rule kprime_IA

Rule kprime_IA is an assignment rule for parameter kprime_IA:

$$\text{kprime\_IA} = \text{K\_IA} \cdot \text{k\_IA} \tag{2}$$

6.3 Rule kprime_II

Rule kprime_II is an assignment rule for parameter kprime_II:

$$\text{kprime\_II} = \text{K\_II} \cdot \text{k\_II} \tag{3}$$

6.4 Rule aux_basal

Rule aux_basal is an assignment rule for parameter aux_basal:

$$\text{aux\_basal} = \frac{1}{\text{K\_aux} \cdot (\text{gamma\_I} - 1)} \tag{4}$$

7 Reactions

This model contains twelve 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	reac_DIA	reac_DIA	$A + I \rightleftharpoons D\_IA$	0000526
2	reac_DII	reac_DII	$I + I \rightleftharpoons D\_II$	0000526
3	reac_degrI	reac_degrI	$I \xrightarrow{aux} \emptyset$	0000179
4	reac_degrA	reac_degrA	$A \longrightarrow \emptyset$	0000179
5	reac_degrDIA	reac_degrDIA	$D\_IA \longrightarrow \emptyset$	0000179
6	reac_degrDII	reac_degrDII	$D\_II \longrightarrow \emptyset$	0000179
7	reac_DIAxA	reac_DIAxA	$D\_IA \xrightarrow{aux} A$	0000180
8	reac_DIIxI	reac_DIIxI	$D\_II \xrightarrow{aux} I$	0000180
9	reac_degrR	reac_degrR	$R \longrightarrow \emptyset$	0000179
10	reac_prodI	reac_prodI	$\emptyset \xrightarrow{R} I$	0000393
11	reac_prodA	reac_prodA	$\emptyset \longrightarrow A$	0000393
12	reac_prodR	reac_prodR	$\emptyset \xrightarrow{A,\ D\_IA,\ I} R$	0000393

7.1 Reaction reac_DIA

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

Name reac_DIA

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{A} + \mathrm{I} \rightleftharpoons \mathrm{D\_IA} \tag{5}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
A	ARF	
I	Aux/IAA	

Product

Table 7: Properties of each product.

Id	Name	SBO
D_IA	Aux/IAA:ARF	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{k\_IA} \cdot [\mathrm{I}] \cdot [\mathrm{A}] - \mathrm{kprime\_IA} \cdot [\mathrm{D\_IA}] \tag{6}$$

7.2 Reaction reac_DII

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

Name reac_DII

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{I} + \mathrm{I} \rightleftharpoons \mathrm{D\_II} \tag{7}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
I	Aux/IAA	
I	Aux/IAA	

Product

Table 9: Properties of each product.

Id	Name	SBO
D_II	Aux/IAA:Aux/IAA	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{k\_II} \cdot [\text{I}] \cdot [\text{I}] - \text{kprime\_II} \cdot [\text{D\_II}] \tag{8}$$

7.3 Reaction reac_degrI

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

Name reac_degrI

SBO:0000179 degradation

Reaction equation

$$\text{I} \xrightarrow{\text{aux}} \emptyset \tag{9}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
I	Aux/IAA	

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
aux	auxin	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\text{gamma\_I} \cdot \text{d\_I} \cdot \text{K\_aux} \cdot [\text{aux}]}{\text{K\_aux} \cdot [\text{aux}] + 1} \cdot [\text{I}] \tag{10}$$

7.4 Reaction reac_degrA

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

Name reac_degrA

SBO:0000179 degradation

Reaction equation

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

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
A	ARF	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{d\_A} \cdot [\text{A}] \tag{12}$$

7.5 Reaction reac_degrDIA

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

Name reac_degrDIA

SBO:0000179 degradation

Reaction equation

$$\text{D\_IA} \longrightarrow \emptyset \tag{13}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
D_IA	Aux/IAA:ARF	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{d\_IA} \cdot [\text{D\_IA}] \tag{14}$$

7.6 Reaction reac_degrDII

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

Name reac_degrDII

SBO:0000179 degradation

Reaction equation

$$\text{D\_II} \longrightarrow \emptyset \tag{15}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
D_II	Aux/IAA:Aux/IAA	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{d\_II} \cdot [\text{D\_II}] \tag{16}$$

7.7 Reaction reac_DIAxA

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

Name reac_DIAxA

SBO:0000180 dissociation

Reaction equation

$$\mathrm{D\_IA} \xrightarrow{\mathrm{aux}} \mathrm{A} \tag{17}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
D_IA	Aux/IAA:ARF	

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
aux	auxin	

Product

Table 17: Properties of each product.

Id	Name	SBO
A	ARF	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\mathrm{gamma\_I} \cdot \mathrm{d\_I} \cdot \mathrm{K\_aux} \cdot [\mathrm{aux}]}{\mathrm{K\_aux} \cdot [\mathrm{aux}] + 1} \cdot [\mathrm{D\_IA}] \tag{18}$$

7.8 Reaction reac_DIIxI

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

Name reac_DIIxI

SBO:0000180 dissociation

Reaction equation

$$\mathrm{D\_II} \xrightarrow{\mathrm{aux}} \mathrm{I} \tag{19}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
D_II	Aux/IAA:Aux/IAA	

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
aux	auxin	

Product

Table 20: Properties of each product.

Id	Name	SBO
I	Aux/IAA	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\mathrm{gamma\_I} \cdot \mathrm{d\_I} \cdot \mathrm{K\_aux} \cdot [\mathrm{aux}]}{\mathrm{K\_aux} \cdot [\mathrm{aux}] + 1} \cdot [\mathrm{D\_II}] \tag{20}$$

7.9 Reaction reac_degrR

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

Name reac_degrR

SBO:0000179 degradation

Reaction equation

$$\mathrm{R} \longrightarrow \emptyset \tag{21}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
R	mRNA	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{d\_r} \cdot [\mathrm{R}] \tag{22}$$

7.10 Reaction reac_prodI

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

Name reac_prodI

SBO:0000393 production

Reaction equation

$$\emptyset \xrightarrow{\mathrm{R}} \mathrm{I} \tag{23}$$

Modifier

Table 22: Properties of each modifier.

Id	Name	SBO
R	mRNA	

Product

Table 23: Properties of each product.

Id	Name	SBO
I	Aux/IAA	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{pi\_I} \cdot [\text{R}] \tag{24}$$

7.11 Reaction reac_prodA

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

Name reac_prodA

SBO:0000393 production

Reaction equation

$$\emptyset \longrightarrow \text{A} \tag{25}$$

Product

Table 24: Properties of each product.

Id	Name	SBO
A	ARF	

Kinetic Law

Derived unit not available

$$v_{11} = \text{pi\_A} \tag{26}$$

7.12 Reaction reac_prodR

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

Name reac_prodR

SBO:0000393 production

Reaction equation

$$\emptyset \xrightarrow{\text{A, D\_IA, I}} \text{R} \tag{27}$$

Modifiers

Table 25: Properties of each modifier.

Id	Name	SBO
A	ARF	
D_IA	Aux/IAA:ARF	
I	Aux/IAA	

Product

Table 26: Properties of each product.

Id	Name	SBO
R	mRNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \frac{1 + \frac{\text{f\_c}}{\text{B\_d}} \cdot [\text{A}] \cdot \left(1 + \frac{\text{w\_A} \cdot \text{f\_A} \cdot [\text{A}]}{\text{B\_d}}\right)}{1 + \frac{[\text{A}]}{\text{B\_d}} \cdot \left(1 + \frac{\text{w\_A} \cdot [\text{A}]}{\text{B\_d}}\right) + \frac{\text{w\_I} \cdot [\text{A}] \cdot [\text{I}]}{\text{K\_IA} \cdot \text{B\_d}} + \frac{\text{w\_D} \cdot [\text{D\_IA}]}{\text{B\_d}} + \text{k\_Am}} \tag{28}$$

8 Derived Rate Equations

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

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

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

8.1 Species I

Name Aux/IAA

SBO:0000252 polypeptide chain

Initial concentration $10\ \text{mol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in reac_DIA, reac_DII, reac_DII, reac_degrI and as a product in reac_DIIxI, reac_prodI and as a modifier in reac_prodR).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{I} = v_8 + v_{10} - v_1 - v_2 - v_2 - v_3 \tag{29}$$

8.2 Species A

Name ARF

SBO:0000252 polypeptide chain

Initial concentration $10\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in reac_DIA, reac_degrA and as a product in reac_DIAxA, reac_prodA and as a modifier in reac_prodR).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} = v_7 + v_{11} - v_1 - v_4 \tag{30}$$

8.3 Species D_II

Name Aux/IAA:Aux/IAA

SBO:0000286 multimer

Initial concentration $10\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in reac_degrDII, reac_DIIxI and as a product in reac_DII).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{D\_II} = v_2 - v_6 - v_8 \tag{31}$$

8.4 Species D_IA

Name Aux/IAA:ARF

SBO:0000297 protein complex

Initial concentration $10\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in reac_degrDIA, reac_DIAxA and as a product in reac_DIA and as a modifier in reac_prodR).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{D\_IA} = v_1 - v_5 - v_7 \tag{32}$$

8.5 Species R

Name mRNA

SBO:0000278 messenger RNA

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

This species takes part in three reactions (as a reactant in reac_degrR and as a product in reac_prodR and as a modifier in reac_prodI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R} = v_{12} - v_9 \tag{33}$$

8.6 Species aux

Name auxin

SBO:0000252 polypeptide chain

Initial concentration $0.11\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

Involved in rule aux

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

A Glossary of Systems Biology Ontology Terms

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

SBO:0000153 forward rate constant: Numerical parameter that quantifies the forward velocity of a chemical reaction. This parameter encompasses all the contributions to the velocity except the quantity of the reactants

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

SBO:0000286 multimer: Non-covalent association of identical, or pseudo-identical, entities. By pseudo-identical entities, we mean biochemical elements that differ chemically, although remaining globally identical in structure and/or function. Examples are homologous subunits in an hetero-oligomeric receptor

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:0000338 dissociation rate constant: Rate with which a complex dissociates into its components

SBO:0000341 association rate constant: Rate with which components associate into a complex

SBO:0000356 decay constant: Kinetic constant characterising a mono-exponential decay. It is the inverse of the mean lifetime of the continuant being decayed. Its unit is"per tim".

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

SBO:0000481 stoichiometric coefficient: The stoichiometric coefficient represents the degree to which a chemical species participates in a reaction. It corresponds to the number of molecules of a reactant that are consumed or produced with each occurrence of a reaction event

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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