SBML Model Report

Model name: “Ouyang2014 - photomorphogenic UV-B signalling network”

September 10, 2014

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 Xinhao Ouyang[2] at September fourth 2014 at 12:37 a. m. and last time modified at September fourth 2014 at 2:22 p. m. Table 1 provides an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	14
events	0	constraints	0
reactions	10	function definitions	0
global parameters	25	unit definitions	0
rules	2	initial assignments	0

Model Notes

Ouyang2014 - photomorphogenic UV-B signallingnetwork

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This model is described in the article:Coordinated photomorphogenic UV-B signaling network captured by mathematical modeling.Ouyang X, Huang X, Jin X, Chen Z, Yang P, Ge H, Li S, Deng XW.Proc. Natl. Acad. Sci. U.S.A. 2014 Aug; 111(31): 11539-11544

Abstract:

Long-wavelength and low-fluence UV-B light is an informational signal known to induce photomorphogenic development in plants. Using the model plant Arabidopsis thaliana, a variety of factors involved in UV-B-specific signaling have been experimentally characterized over the past decade, including the UV-B light receptor UV resistance locus 8; the positive regulators constitutive photomorphogenesis 1 and elongated hypocotyl 5; and the negative regulators cullin4, repressor of UV-B photomorphogenesis 1 (RUP1), and RUP2. Individual genetic and molecular studies have revealed that these proteins function in either positive or negative regulatory capacities for the sufficient and balanced transduction of photomorphogenic UV-B signal. Less is known, however, regarding how these signaling events are systematically linked. In our study, we use a systems biology approach to investigate the dynamic behaviors and correlations of multiple signaling components involved in Arabidopsis UV-B-induced photomorphogenesis. We define a mathematical representation of photomorphogenic UV-B signaling at a temporal scale. Supplemented with experimental validation, our computational modeling demonstrates the functional interaction that occurs among different protein complexes in early and prolonged response to photomorphogenic UV-B.

This model is hosted on BioModels Database and identified by: BIOMD0000000545.

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 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
`Hypctol`	Hypctol		3	1	litre	☑	

3.1 Compartment `Hypctol`

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

Name Hypctol

4 Species

This model contains 14 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
CS	CS	Hypctol	mol	⊟	⊟
CD	CD	Hypctol	mol	⊟	⊟
CDCS	CDCS	Hypctol	mol	⊟	⊟
UVR8M	UVR8M	Hypctol	mol	⊟	⊟
UCS	UCS	Hypctol	mol	⊟	⊟
UVR8D	UVR8D	Hypctol	mol	⊟	⊟
RUP	RUP	Hypctol	mol	⊟	⊟
UR	UR	Hypctol	mol	⊟	⊟
UVR8_M	UVR8_M	Hypctol	mol	⊟	⊟
COP1	COP1	Hypctol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
HY5	HY5	Hypctol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
FHY3	FHY3	Hypctol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	⊟
DWD	DWD	Hypctol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CDW	CDW	Hypctol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 25 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ks1	ks1		0.230		☑
ks2	ks2		4.053		☑
kdr1	kdr1		0.100		☑
kdr2	kdr2		0.212		☑
k1	k1		0.004		☑
k2	k2		161.620		☑
ka1	ka1		0.037		☑
ka2	ka2		0.061		☑
ka3	ka3		4.721		☑
kd1	kd1		94.352		☑
kd2	kd2		50.697		☑
kd3	kd3		0.551		☑
ks3	ks3		0.440		☑
kdr3	kdr3		1.246		☑
UV	UV		1.000		☑
ka4	ka4		10.129		☑
kd4	kd4		1.200		☑
n1	n1		3.000		☑
n2	n2		2.000		☑
n3	n3		3.500		☑
kdr3a	kdr3a		0.974		☑
kdr3b	kdr3b		0.406		☑
ksr	ksr		0.754		☑
UM_Total	UM_Total		0.000		☐
COP1_Total	COP1_Total		0.000		☐

6 Rules

This is an overview of two rules.

6.1 Rule UM_Total

Rule UM_Total is an assignment rule for parameter UM_Total:

$$\text{UM\_Total} = 2 \cdot \text{UCS} + \text{UVR8M} + \text{UR} \tag{1}$$

6.2 Rule COP1_Total

Rule COP1_Total is an assignment rule for parameter COP1_Total:

$$\text{COP1\_Total} = 2 \cdot \text{UCS} + 2 \cdot \text{CDCS} + \text{CS} \tag{2}$$

7 Reactions

This model contains ten 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	r1		$\emptyset \xrightarrow{\text{HY5, FHY3, HY5, FHY3, CS}} \text{CS}$	
2	r2		$\emptyset \xrightarrow{\text{UCS, UCS, RUP}} \text{RUP}$	
3	r3		$2\,\text{UVR8M} \xrightarrow{\text{UVR8M}} \text{UVR8D}$	
4	r4		$2\,\text{CS} + 2\,\text{UVR8M} \xrightleftharpoons{\text{CS, UVR8M, UCS}} \text{UCS}$	
5	r5		$2\,\text{CS} + \text{CD} \xrightleftharpoons{\text{CS, CD, CDCS}} \text{CDCS}$	
6	r6		$\text{UVR8M} + \text{RUP} \xrightarrow{\text{UVR8M, RUP}} \text{UR}$	
7	r7		$2\,\text{UR} \xrightarrow{\text{UR}} \text{UVR8D} + 2\,\text{RUP}$	
8	r8		$\text{UVR8D} \xrightarrow{\text{UVR8D}} 2\,\text{UVR8M}$	
9	r9		$\emptyset \xrightarrow{\text{CDCS, CDW, UCS, CDCS, CDW, UCS, HY5}} \text{HY5}$	
10	r10		$\text{CD} + \text{DWD} \xrightleftharpoons{\text{CD, DWD, CDW}} \text{CDW}$	

7.1 Reaction r1

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

Reaction equation

$$\emptyset \xrightarrow{\text{HY5, FHY3, HY5, FHY3, CS}} \text{CS} \tag{3}$$

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
HY5	HY5	
FHY3	FHY3	
HY5	HY5	
FHY3	FHY3	
CS	CS	

Product

Table 7: Properties of each product.

Id	Name	SBO
CS	CS	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{ks1} \cdot (1 + \text{UV} \cdot \text{n3} \cdot ([\text{HY5}] + [\text{FHY3}])) - \text{kdr1} \cdot (1 + \text{n1} \cdot \text{UV}) \cdot \text{CS} \tag{4}$$

7.2 Reaction r2

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

Reaction equation

$$\emptyset \xrightarrow{\text{UCS, UCS, RUP}} \text{RUP} \tag{5}$$

Modifiers

Table 8: Properties of each modifier.

Id	Name	SBO
UCS	UCS	
UCS	UCS	
RUP	RUP	

Product

Table 9: Properties of each product.

Id	Name	SBO
RUP	RUP	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{ks2} \cdot (1 + \mathrm{UV} \cdot \mathrm{UCS}) - \mathrm{kdr2} \cdot \mathrm{RUP} \tag{6}$$

7.3 Reaction r3

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

Reaction equation

$$2\,\mathrm{UVR8M} \xrightarrow{\mathrm{UVR8M}} \mathrm{UVR8D} \tag{7}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
UVR8M	UVR8M	

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
UVR8M	UVR8M	

Product

Table 12: Properties of each product.

Id	Name	SBO
UVR8D	UVR8D	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{k1} \cdot \mathrm{UVR8M}^2 \tag{8}$$

7.4 Reaction r4

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

Reaction equation

$$2\,\mathrm{CS} + 2\,\mathrm{UVR8M} \xrightleftharpoons{\text{CS, UVR8M, UCS}} \mathrm{UCS} \tag{9}$$

Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
CS	CS	
UVR8M	UVR8M	

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
CS	CS	
UVR8M	UVR8M	
UCS	UCS	

Product

Table 15: Properties of each product.

Id	Name	SBO
UCS	UCS	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{ka1} \cdot \mathrm{CS}^2 \cdot \mathrm{UVR8M}^2 - \mathrm{kd1} \cdot \mathrm{UCS} \tag{10}$$

7.5 Reaction r5

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

Reaction equation

$$2\,\mathrm{CS} + \mathrm{CD} \xrightleftharpoons{\text{CS, CD, CDCS}} \mathrm{CDCS} \tag{11}$$

Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
CS	CS	
CD	CD	

Modifiers

Table 17: Properties of each modifier.

Id	Name	SBO
CS	CS	
CD	CD	
CDCS	CDCS	

Product

Table 18: Properties of each product.

Id	Name	SBO
CDCS	CDCS	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{ka2} \cdot \mathrm{CS}^2 \cdot \mathrm{CD} - \mathrm{kd2} \cdot \mathrm{CDCS} \tag{12}$$

7.6 Reaction r6

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

Reaction equation

$$\mathrm{UVR8M} + \mathrm{RUP} \xrightarrow{\mathrm{UVR8M,\ RUP}} \mathrm{UR} \tag{13}$$

Reactants

Table 19: Properties of each reactant.

Id	Name	SBO
UVR8M	UVR8M	
RUP	RUP	

Modifiers

Table 20: Properties of each modifier.

Id	Name	SBO
UVR8M	UVR8M	
RUP	RUP	

Product

Table 21: Properties of each product.

Id	Name	SBO
UR	UR	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{ka3} \cdot \mathrm{UVR8M} \cdot \mathrm{RUP} \tag{14}$$

7.7 Reaction r7

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

Reaction equation

$$2\,\mathrm{UR} \xrightarrow{\mathrm{UR}} \mathrm{UVR8D} + 2\,\mathrm{RUP} \tag{15}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
UR	UR	

Modifier

Table 23: Properties of each modifier.

Id	Name	SBO
UR	UR	

Products

Table 24: Properties of each product.

Id	Name	SBO
UVR8D	UVR8D	
RUP	RUP	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{kd3} \cdot \mathrm{UR}^2 \tag{16}$$

7.8 Reaction r8

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

Reaction equation

$$\mathrm{UVR8D} \xrightarrow{\mathrm{UVR8D}} 2\,\mathrm{UVR8M} \tag{17}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
UVR8D	UVR8D	

Modifier

Table 26: Properties of each modifier.

Id	Name	SBO
UVR8D	UVR8D	

Product

Table 27: Properties of each product.

Id	Name	SBO
UVR8M	UVR8M	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{k2} \cdot \mathrm{UVR8D} \tag{18}$$

7.9 Reaction r9

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

Reaction equation

$$\emptyset \xrightarrow{\text{CDCS, CDW, UCS, CDCS, CDW, UCS, HY5}} \text{HY5} \tag{19}$$

Modifiers

Table 28: Properties of each modifier.

Id	Name	SBO
CDCS	CDCS	
CDW	CDW	
UCS	UCS	
CDCS	CDCS	
CDW	CDW	
UCS	UCS	
HY5	HY5	

Product

Table 29: Properties of each product.

Id	Name	SBO
HY5	HY5	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{ks3} \cdot (1 + \text{n2} \cdot \text{UV}) - \text{kdr3} \cdot \left(\frac{\text{CDCS}}{\text{kdr3a} + \text{CDCS}} + \frac{[\text{CDW}]}{\text{kdr3b} + [\text{CDW}]} - \frac{\text{UCS}}{\text{ksr} + \text{UCS}} \right) \cdot [\text{HY5}] \tag{20}$$

7.10 Reaction r10

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

Reaction equation

$$\text{CD} + \text{DWD} \xrightleftharpoons{\text{CD, DWD, CDW}} \text{CDW} \tag{21}$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
CD	CD	
DWD	DWD	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
CD	CD	
DWD	DWD	
CDW	CDW	

Product

Table 32: Properties of each product.

Id	Name	SBO
CDW	CDW	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{ka4} \cdot \text{CD} \cdot [\text{DWD}] - \text{kd4} \cdot [\text{CDW}] \tag{22}$$

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 CS

Name CS

Initial amount 0.2 mol

This species takes part in six reactions (as a reactant in r4, r5 and as a product in r1 and as a modifier in r1, r4, r5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CS} = v_1 - 2\,v_4 - 2\,v_5 \tag{23}$$

8.2 Species CD

Name CD

Initial amount 10 mol

This species takes part in four reactions (as a reactant in r5, r10 and as a modifier in r5, r10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CD} = -v_5 - v_{10} \tag{24}$$

8.3 Species CDCS

Name CDCS

Initial amount 2 mol

This species takes part in four reactions (as a product in r5 and as a modifier in r5, r9, r9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CDCS} = v_5 \tag{25}$$

8.4 Species UVR8M

Name UVR8M

Initial amount 0 mol

This species takes part in seven reactions (as a reactant in r3, r4, r6 and as a product in r8 and as a modifier in r3, r4, r6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UVR8M} = 2\,v_8 - 2\,v_3 - 2\,v_4 - v_6 \tag{26}$$

8.5 Species UCS

Name UCS

Initial amount 0 mol

This species takes part in six reactions (as a product in r4 and as a modifier in r2, r2, r4, r9, r9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UCS} = v_4 \tag{27}$$

8.6 Species UVR8D

Name UVR8D

Initial amount 20 mol

This species takes part in four reactions (as a reactant in r8 and as a product in r3, r7 and as a modifier in r8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UVR8D} = v_3 + v_7 - v_8 \tag{28}$$

8.7 Species RUP

Name RUP

Initial amount 0 mol

This species takes part in five reactions (as a reactant in r6 and as a product in r2, r7 and as a modifier in r2, r6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{RUP} = v_2 + 2\,v_7 - v_6 \tag{29}$$

8.8 Species UR

Name UR

Initial amount 0 mol

This species takes part in three reactions (as a reactant in r7 and as a product in r6 and as a modifier in r7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UR} = v_6 - 2\,v_7 \tag{30}$$

8.9 Species UVR8_M

Name UVR8_M

Initial amount 0 mol

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UVR8\_M} = 0 \tag{31}$$

8.10 Species COP1

Name COP1

Initial amount 4.2 mol

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{COP1} = 0 \tag{32}$$

8.11 Species HY5

Name HY5

Initial amount 0.25 mol

This species takes part in four reactions (as a product in r9 and as a modifier in r1, r1, r9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{HY5} = v_9 \tag{33}$$

8.12 Species FHY3

Name FHY3

Initial amount 5 mol

This species takes part in two reactions (as a modifier in r1, r1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FHY3} = 0 \tag{34}$$

8.13 Species DWD

Name DWD

Initial amount 20 mol

This species takes part in two reactions (as a reactant in r10 and as a modifier in r10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DWD} = -v_{10} \tag{35}$$

8.14 Species CDW

Name CDW

Initial amount 0 mol

This species takes part in four reactions (as a product in r10 and as a modifier in r9, r9, r10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CDW} = v_{10} \tag{36}$$

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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