# **SBML Model Report**

# Model name: "Valero2016 Ascorbate-Glutathione cycle in chloroplasts under light/dark conditions"



February 22, 2017

#### 1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following eight authors: Nick Juty<sup>1</sup>, Vijayalakshmi Chelliah<sup>2</sup>, Edelmira Valero<sup>3</sup>, Francisco Garca-Carmona<sup>4</sup>, Jos Antonio Hernndez<sup>5</sup>, Ildefonso De La Fuente<sup>6</sup>, Mara Isabel Gonzlez-Snchez<sup>7</sup> and Hermenegilda Maci<sup>8</sup> at September 27<sup>th</sup> 2011 at 11:15 a.m. and last time modified at March 17<sup>th</sup> 2016 at 1:13 p.m. Table 1 provides an overview of the quantities of all components of this model.

#### **Model Notes**

Valero2016 - Ascorbate-Glutathione cycle in chloroplasts under light/dark conditions

This model is described in the article: Modeling the ascorbate-glutathione cycle in chloroplasts
under light/dark conditions. Valero E, Maci H, De la Fuente IM, Hernndez JA, Gonzlez-Snchez
MI, Garca-Carmona F. BMC Syst Biol 2016; 10(1): 11

Abstract:

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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	13
events	0	constraints	0
reactions	0	function definitions	1
global parameters	68	unit definitions	2
rules	29	initial assignments	17

Light/dark cycles are probably the most important environmental signals that regulate plant development. Light is essential for photosynthesis, but an excess, in combination with the unavoidable presence of atmospheric oxygen inside the chloroplast, leads to excessive reactive oxygen species production. Among the defense mechanisms that activate plants to cope with environmental stress situations, it is worth noting the ascorbate-glutathione cycle, a complex metabolic pathway in which a variety of photochemical, chemical and enzymatic steps are involved. We herein studied the dynamic behavior of this pathway under light/dark conditions and for several consecutive days. For this purpose, a mathematical model was developed including a variable electron source with a rate law proportional to the intensity of solar irradiance during the photoperiod, and which is continuously turned off at night and on again the next day. The model is defined by a nonlinear system of ordinary differential equations with an on/off timedependent input, including a parameter to simulate the fact that the photoperiod length is not constant throughout the year, and which takes into account the particular experimental kinetics of each enzyme involved in the pathway. Unlike previous models, which have only provided steady-state solutions, the present model is able to simulate diurnal fluctuations in the metabolite concentrations, fluxes and enzymatic rates involved in the network. The obtained results are broadly consistent with experimental observations and highlight the key role played by ascorbate recycling for plants to adapt to their surrounding environment. This approach provides a new strategy to in vivo studies to analyze plant defense mechanisms against oxidative stress induced by external changes, which can also be extrapolated to other complex metabolic pathways to constitute a useful tool to the scientific community in general.

This model is hosted on BioModels Database and identified by: BIOMD0000000589.

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

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#### 2 Unit Definitions

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

#### 2.1 Unit time

Name time

**Definition** 3600 s

#### 2.2 Unit substance

Name substance

**Definition** µmol

#### 2.3 Unit volume

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

**Definition** 1

#### 2.4 Unit area

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

**Definition** m<sup>2</sup>

# 2.5 Unit length

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

**Definition** m

# 3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
С	c	0000290	3	1	litre	Ø	

# **3.1 Compartment** c

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

Name c

SBO:0000290 physical compartment

4

# 4 Species

This model contains 13 species. The boundary condition of 13 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
					Condi- tion
NADPH	NADPH	С	$\mu$ mol·l <sup>-1</sup>		<u> </u>
NADPplus	NADPplus	С	$\mu \text{mol} \cdot l^{-1}$		$\mathbf{Z}$
GSH	GSH	С	$\mu$ mol·l <sup>-1</sup>	$\Box$	$\overline{\mathbf{Z}}$
GSSG	GSSG	С	$\mu$ mol·l <sup>-1</sup>	$\Box$	
ASC	ASC	С	$\mu mol \cdot l^{-1}$	$\Box$	
DHA	DHA	С	$\mu \mathrm{mol} \cdot \mathrm{l}^{-1}$	$\Box$	
MDA	MDA	С	$\mu \mathrm{mol} \cdot \mathrm{l}^{-1}$	$\Box$	
H202	H2O2	С	$\mu \mathrm{mol} \cdot \mathrm{l}^{-1}$	$\Box$	
APX	APX	С	$\mu mol \cdot l^{-1}$	$\Box$	
CoI	CoI	С	$\mu mol \cdot l^{-1}$		
CoII	CoII	С	$\mu mol \cdot l^{-1}$	$\Box$	
APXi	APXi	С	$\mu mol \cdot l^{-1}$	$\Box$	$\overline{\mathbf{Z}}$
02neg	O2neg	С	$\mu mol \cdot l^{-1}$	$\Box$	

# **5 Parameters**

This model contains 68 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO V	Value	Unit	Constant
vGR	vGR		0.000		
vDHAR	vDHAR		0.000		
vSOD	vSOD		0.000		
F12	F12	7.95693107	$7900941 \cdot 10^{-10}$		
k12	k12	2	2200.000		
kN	kN	3.97846553	$3950471 \cdot 10^{-12}$		
k4	k4	2	2520.000		
k3	k3		0.010		$\overline{\checkmark}$
F13	F13		0.000		
kSOD	kSOD	720	000.000		$\mathbf{Z}$
SOD	SOD		50.000		
kcatDHAR	kcatDHAR	511	200.000		$   \overline{\mathscr{L}} $
DHAR	DHAR		1.700		$\square$
K	K		500.000		$   \overline{\mathscr{A}} $
KMDHA	KM_DHAR_DHA		70.000		$   \overline{\mathscr{L}} $
KMGSH	KM_DHAR_GSH	2	2500.000		$   \overline{\mathscr{L}} $
k1	k1	1	800.000		$\square$
k13	k13	15	5000.000		$\square$
k2APX	k2APX	180	000.000		$\square$
k3APX	k3APX	7	7560.000		$\square$
k4APX	k4APX	2	2520.000		$   \overline{\mathscr{A}} $
k5APX	k5APX		1.000		
k6	k6		720.000		
k5	k5		0.007		$\square$
k1APX	k1APX	43	3200.000		
k2	k2		720.000		
F1	F1	9.31322574	$4615479 \cdot 10^{-10}$		
F11	F11	1.35629466	$6714537 \cdot 10^{-10}$		
GR	GR		1.400		$\mathbf{Z}$
kcatGR	kcatGR	2142	2000.000		
KMNADPH	KM-GR_NADPH		3.000		
KMGSSG	KM_GR_GSSG		200.000		$\square$
k11	k11		000.000		$\checkmark$
a1	a1	4022	2883.370		
b	b		11.000		
c_0	c		4.712		
c11	c11		0.146		

Id	Name	SBO	Value	Unit	Constant
c12	c12		0.854		
c13	c13		0.000		
a2	a2		3895707.971		
incr	incr		0.250		$ \overline{\checkmark} $
a3	a3		4461050.658		
a4	a4		4143378.612	•	$\square$
<b>a</b> 5	a5		3793894.049	1	
a6	a6		4190686.199	1	$\square$
a7	a7		3699605.442	,	
a8	a8		3867960.799	1	$\square$
a9	a9		4156529.255		$\square$
a10	a10		3632875.100	)	
a11	a11		3901158.197	,	
a12	a12		3938901.525		$\square$
a13	a13		3614615.748		
a14	a14		3540932.604	•	
a0	a0		4431968.607	,	<b>⊉</b> ⊟
i	i		0.000		
kNcte	kN_cte		0.005		
ai	ai		4431968.607	,	
a15	a15		4445756.614		
min	min		3500000.000		
max	max		4500000.000		
FN	FN	4	1.376313394255		
vAPX	vAPX		0.000		
MDAR	MDAR		0.000		
kcatMDAR	kcatMDAR		1080000.000		
KMNADPH2	KM-MDAR- _NADPH		23.000		$\square$
KMMDA	KM_MDAR_MDA		1.400	)	
vMDAR	vMDAR		0.000		
Metabolite- _17	Initial for APX		40.000		

# 6 Initialassignments

This is an overview of 17 initial assignments.

# **6.1 Initialassignment** a1

**Derived unit** contains undeclared units

#### **Math** RUNIFORM (min, max)

# **6.2 Initialassignment** a2

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

## 6.3 Initialassignment a3

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

# **6.4 Initialassignment** a4

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

#### 6.5 Initialassignment a5

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

#### **6.6 Initialassignment** a6

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

#### **6.7 Initialassignment** a7

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

#### 6.8 Initialassignment a8

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

## 6.9 Initialassignment a9

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

#### 6.10 Initialassignment a10

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

## 6.11 Initialassignment a11

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

# 6.12 Initialassignment a12

Derived unit contains undeclared units

**Math** RUNIFORM (min, max)

# 6.13 Initialassignment a13

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

#### 6.14 Initialassignment a14

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

#### 6.15 Initialassignment a0

**Derived unit** contains undeclared units

**Math** RUNIFORM (min, max)

# 6.16 Initialassignment a15

Derived unit contains undeclared units

**Math** RUNIFORM (min, max)

#### **6.17 Initialassignment Metabolite\_17**

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

Math [APX]

#### 7 Function definition

This is an overview of one function definition.

#### 7.1 Function definition RUNIFORM

Arguments a, b

## **Mathematical Expression**

$$\frac{a+b}{2} \tag{1}$$

#### 8 Rules

This is an overview of 29 rules.

#### 8.1 Rule vGR

Rule vGR is an assignment rule for parameter vGR:

$$vGR = \frac{kcatGR \cdot GR \cdot [NADPH] \cdot [GSSG]}{KMNADPH \cdot [GSSG] + KMGSSG \cdot [NADPH] + [NADPH] \cdot [GSSG]} \tag{2}$$

#### 8.2 Rule vDHAR

Rule vDHAR is an assignment rule for parameter vDHAR:

$$vDHAR = \frac{kcatDHAR \cdot DHAR \cdot [DHA] \cdot [GSH]}{K + KMDHA \cdot [GSH] + KMGSH \cdot [DHA] + [DHA] \cdot [GSH]}$$
 (3)

#### 8.3 Rule vSOD

Rule vSOD is an assignment rule for parameter vSOD:

$$vSOD = kSOD \cdot SOD \cdot [O2neg] \tag{4}$$

#### **8.4 Rule** c13

Rule c13 is an assignment rule for parameter c13:

$$c13 = \frac{k13 \cdot [MDA]}{k11 + 2 \cdot k12 \cdot [NADPplus] + k13 \cdot [MDA]}$$
 (5)

#### 8.5 Rule c11

Rule c11 is an assignment rule for parameter c11:

$$c11 = \frac{k11}{k11 + 2 \cdot k12 \cdot [NADPplus] + k13 \cdot [MDA]}$$
 (6)

#### **8.6 Rule** c12

Rule c12 is an assignment rule for parameter c12:

$$c12 = \frac{2 \cdot k12 \cdot [NADPplus]}{k11 + 2 \cdot k12 \cdot [NADPplus] + k13 \cdot [MDA]}$$
 (7)

# 8.7 Rule i

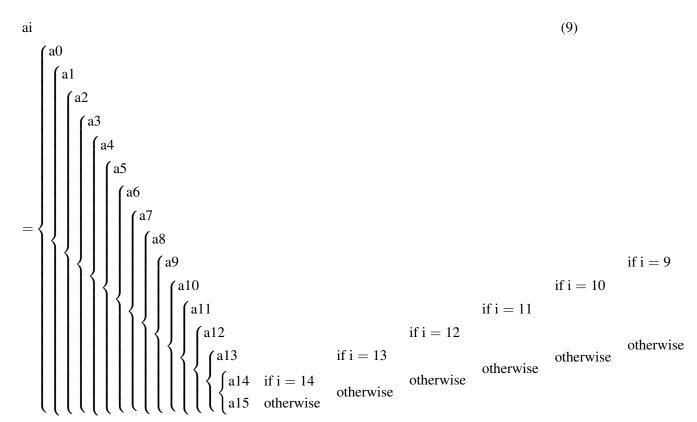
Rule i is an assignment rule for parameter i:

$$i = \left\lfloor \frac{\text{time}}{24} \right\rfloor \tag{8}$$

Derived unit 3600 s

#### 8.8 Rule ai

Rule ai is an assignment rule for parameter ai:



#### 8.9 Rule F1

Rule F1 is an assignment rule for parameter F1:

$$\begin{aligned} & F1 \\ &= \begin{cases} ai + ai \cdot sin \left( \frac{2 \cdot \pi \cdot (time - i \cdot 24)}{b + incr \cdot i} + c \text{\_}0 \right) & \text{if } (time \geq i \cdot 24) \land (time \leq i \cdot 24 + b + incr \cdot i) \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

#### **8.10 Rule** F12

Rule F12 is an assignment rule for parameter F12:

$$F12 = c12 \cdot F1 \tag{11}$$

#### 8.11 Rule kN

Rule kN is an assignment rule for parameter kN:

$$kN = kN_{c}te \cdot F12 \tag{12}$$

#### 8.12 Rule F13

Rule F13 is an assignment rule for parameter F13:

$$F13 = c13 \cdot F1 \tag{13}$$

#### **8.13 Rule** F11

Rule F11 is an assignment rule for parameter F11:

$$F11 = c11 \cdot F1 \tag{14}$$

#### **8.14 Rule FN**

Rule FN is an assignment rule for parameter FN:

$$FN = kN \cdot [NADPH] \tag{15}$$

#### 8.15 Rule vAPX

Rule vAPX is an assignment rule for parameter vAPX:

$$vAPX = k2APX \cdot [CoI] \cdot [ASC] + k3APX \cdot [CoII] \cdot [ASC]$$
(16)

#### 8.16 Rule vMDAR

Rule vMDAR is an assignment rule for parameter vMDAR:

$$vMDAR = \frac{kcatMDAR \cdot MDAR \cdot [NADPH] \cdot [MDA]}{KMNADPH2 \cdot [MDA] + KMMDA \cdot [NADPH] + [NADPH] \cdot [MDA]}$$
(17)

#### 8.17 Rule NADPH

Rule NADPH is a rate rule for species NADPH:

$$\frac{d}{dt}NADPH = vGR - kN \cdot [NADPH] + F12 \cdot 0.5 - vMDAR$$
 (18)

#### 8.18 Rule NADPplus

Rule NADPplus is a rate rule for species NADPplus:

$$\frac{d}{dt}NADPplus = vGR + kN \cdot [NADPH] - F12 \cdot 0.5 + vMDAR$$
 (19)

#### 8.19 Rule GSH

Rule GSH is a rate rule for species GSH:

$$\frac{d}{dt}GSH = 2 \cdot (vGR - vDHAR - k4 \cdot [O2neg] \cdot [GSH] - k3 \cdot [DHA] \cdot [GSH])$$
 (20)

#### 8.20 Rule GSSG

Rule GSSG is a rate rule for species GSSG:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GSSG} = \mathrm{vGR} + \mathrm{vDHAR} + \mathrm{k4} \cdot [\mathrm{O2neg}] \cdot [\mathrm{GSH}] + \mathrm{k3} \cdot [\mathrm{DHA}] \cdot [\mathrm{GSH}] \tag{21}$$

#### 8.21 Rule ASC

Rule ASC is a rate rule for species ASC:

$$\frac{d}{dt}ASC = vDHAR + k1 \cdot [MDA]^2 + k3 \cdot [DHA] \cdot [GSH] + F13 - k2APX \cdot [ASC] \cdot [CoI] - k3APX$$

$$\cdot [ASC] \cdot [CoII] - k6 \cdot [O2neg] \cdot [ASC] - 2 \cdot k5 \cdot [H2O2] \cdot [ASC] + 2 \cdot vMDAR$$
(22)

## 8.22 Rule DHA

Rule DHA is a rate rule for species DHA:

$$\frac{d}{dt}DHA = vDHAR + k1 \cdot [MDA]^2 - k3 \cdot [DHA] \cdot [GSH]$$
(23)

#### 8.23 Rule MDA

Rule MDA is a rate rule for species MDA:

$$\frac{d}{dt}MDA = k2APX \cdot [ASC] \cdot [CoI] + k3APX \cdot [ASC] \cdot [CoII] - 2 \cdot k1 \cdot [MDA]^{2} + k6 \cdot [O2neg] \cdot [ASC] + 2 \cdot k5 \cdot [H2O2] \cdot [ASC] - F13 - 2 \cdot vMDAR$$
(24)

#### 8.24 Rule H202

Rule H202 is a rate rule for species H202:

$$\frac{d}{dt}H2O2 = vSOD - k1APX \cdot [H2O2] \cdot [APX] - k4APX \cdot [H2O2] \cdot [CoI] + k2 \cdot [O2neg]^2$$

$$+ k6 \cdot [O2neg] \cdot [ASC] + k4 \cdot [O2neg] \cdot [GSH] - k5 \cdot [H2O2] \cdot [ASC]$$
(25)

#### 8.25 Rule APX

Rule APX is a rate rule for species APX:

$$\frac{d}{dt}APX = k1APX \cdot [H2O2] \cdot [APX] + k3APX \cdot [ASC] \cdot [CoII] + k5APX \cdot (Metabolite_17 - [APX] - [CoI] - [CoII])$$
(26)

#### 8.26 Rule CoI

Rule CoI is a rate rule for species CoI:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CoI} = \mathrm{k1APX} \cdot [\mathrm{H2O2}] \cdot [\mathrm{APX}] - \mathrm{k2APX} \cdot [\mathrm{ASC}] \cdot [\mathrm{CoI}] - \mathrm{k4APX} \cdot [\mathrm{H2O2}] \cdot [\mathrm{CoI}] \quad (27)$$

#### 8.27 Rule CoII

Rule CoII is a rate rule for species CoII:

$$\frac{d}{dt}CoII = k2APX \cdot [ASC] \cdot [CoI] - k3APX \cdot [ASC] \cdot [CoII]$$
(28)

#### 8.28 Rule APXi

Rule APXi is a rate rule for species APXi:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{APXi} = \mathrm{k4APX} \cdot [\mathrm{H2O2}] \cdot [\mathrm{CoI}] \tag{29}$$

#### 8.29 Rule 02neg

Rule O2neg is a rate rule for species O2neg:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{O2neg} = 2 \cdot \mathrm{vSOD} + \mathrm{F11} - 2 \cdot \mathrm{k2} \cdot [\mathrm{O2neg}]^2 - \mathrm{k6} \cdot [\mathrm{O2neg}] \cdot [\mathrm{ASC}] - \mathrm{k4} \cdot [\mathrm{O2neg}] \cdot [\mathrm{GSH}] \quad (30)$$

# 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 NADPH

Name NADPH

SBO:0000299 metabolite

Initial concentration  $110.000032696018 \ \mu mol \cdot l^{-1}$ 

Involved in rule NADPH

One rule determines the species' quantity.

# 9.2 Species NADPplus

Name NADPplus

SBO:0000299 metabolite

Notes se ha cambiado las concentraciones iniciales de NADPplus y NADPF

Initial concentration  $40.0000118894612 \ \mu mol \cdot l^{-1}$ 

Involved in rule NADPplus

One rule determines the species' quantity.

# 9.3 Species GSH

Name GSH

SBO:0000299 metabolite

Initial concentration  $4000 \ \mu mol \cdot l^{-1}$ 

Involved in rule GSH

One rule determines the species' quantity.

# 9.4 Species GSSG

Name GSSG

SBO:0000299 metabolite

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

Involved in rule GSSG

One rule determines the species' quantity.

# 9.5 Species ASC

Name ASC

SBO:0000299 metabolite

Initial concentration  $10000~\mu mol \cdot l^{-1}$ 

Involved in rule ASC

One rule determines the species' quantity.

# 9.6 Species DHA

Name DHA

SBO:0000299 metabolite

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

Involved in rule DHA

One rule determines the species' quantity.

# 9.7 Species MDA

Name MDA

SBO:0000299 metabolite

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

Involved in rule MDA

One rule determines the species' quantity.

# **9.8 Species** H202

Name H2O2

SBO:0000247 simple chemical

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

Involved in rule H202

One rule determines the species' quantity.

# 9.9 Species APX

Name APX

**SBO:0000014** enzyme

Initial concentration  $40 \ \mu mol \cdot l^{-1}$ 

Involved in rule APX

One rule determines the species' quantity.

# 9.10 Species CoI

Name CoI

**SBO:0000014** enzyme

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

Involved in rule CoI

One rule determines the species' quantity.

# 9.11 Species CoII

Name CoII

**SBO:0000014** enzyme

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

Involved in rule CoII

One rule determines the species' quantity.

# 9.12 Species APXi

Name APXi

**SBO:0000014** enzyme

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

Involved in rule APXi

One rule determines the species' quantity.

#### 9.13 Species O2neg

Name O2neg

SBO:0000247 simple chemical

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

Involved in rule O2neg

One rule determines the species' quantity.

# A Glossary of Systems Biology Ontology Terms

**SBO:0000014 enzyme:** A protein that catalyzes a chemical reaction. The word comes from en "a" or "i") and simo "leave" or "yeas")

SBO:0000247 simple chemical: Simple, non-repetitive chemical entity

**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:0000299** metabolite: Substance produced by metabolism or by a metabolic process

SBML2LATEX was developed by Andreas Dräger<sup>a</sup>, Hannes Planatscher<sup>a</sup>, Dieudonné M Wouamba<sup>a</sup>, Adrian Schröder<sup>a</sup>, Michael Hucka<sup>b</sup>, Lukas Endler<sup>c</sup>, Martin Golebiewski<sup>d</sup> and Andreas Zell<sup>a</sup>. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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