

SBML Model Report

Model name: “Santolini2001_nNOS- _Mechanism_Regulation”



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following three authors: Lukas Endler¹, Vijayalakshmi Chelliah² and Jrme Santolini³ at October 14th 2008 at 4:56 p. m. and last time modified at April eighth 2016 at 3:56 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	1
species types	0	species	15
events	0	constraints	0
reactions	10	function definitions	0
global parameters	10	unit definitions	4
rules	1	initial assignments	0

Model Notes

This is a model of neuronal Nitric Oxide Synthase expressed in Escherichia coli based on Santolini J. et al. J Biol Chem. (2001) 276(2):1233-43.

Differing from the article, oxygen explicitly included in the reaction 2, 5 and 10 (numbers as

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in scheme 1 in the article). In the article the assumed oxygen concentration of 140 μM was included in the pseudo first order rate constant.

Fig 2E in the article shows different time courses for citrulline and NO than the ones produced by this model. Dr. Santolini, one of the authors of the article, wrote that the legends in fig. 2E might be mixed up and should rather denote NO and NO₃ instead of citrulline and NO.

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2 Unit Definitions

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

2.1 Unit `substance`

Name micromole

Definition μmol

2.2 Unit `peruMpersec`

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

2.3 Unit `uM`

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

2.4 Unit `persec`

Definition s^{-1}

2.5 Unit `volume`

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.6 Unit area

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

Definition m^2

2.7 Unit length

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

Definition m

2.8 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
cytosol			3	1	litre	<input checked="" type="checkbox"/>	

3.1 Compartment cytosol

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

4 Species

This model contains 15 species. The boundary condition of six of these species is set to `true` so that these species' amount cannot be changed by any reaction. 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
FeIII	FeIII	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
FeII	FeII	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
FeII_O2	FeII_O2	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
FeIII_star	FeIII_star	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
FeII_star	FeII_star	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
FeII_star_O2	FeII_star_O2	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
FeIII_NO	FeIII_NO	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
FeII_NO	FeII_NO	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
NADPH	NADPH	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
O2	O2	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
citrulline	citrulline	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
NO3	NO3	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
NO	NO	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
NADPplus	NADPplus	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
FeIII_t	FeIII_t	cytosol	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>

5 Parameters

This model contains ten global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000035	2.600	s^{-1}	<input checked="" type="checkbox"/>
k2	k2	0000339	0.900	$l \cdot \mu\text{mol}^{-1} \cdot s^{-1}$	<input checked="" type="checkbox"/>
k3	k3	0000035	26.000	s^{-1}	<input checked="" type="checkbox"/>
k4	k4	0000035	2.600	s^{-1}	<input checked="" type="checkbox"/>
k5	k5	0000339	0.900	$l \cdot \mu\text{mol}^{-1} \cdot s^{-1}$	<input checked="" type="checkbox"/>
k6	k6	0000035	26.000	s^{-1}	<input checked="" type="checkbox"/>
k7	k7	0000035	5.000	s^{-1}	<input checked="" type="checkbox"/>
k8	k8	0000035	2.600	s^{-1}	<input checked="" type="checkbox"/>
k9	k9	0000035	10^{-4}	s^{-1}	<input checked="" type="checkbox"/>
k10	k10	0000339	0.001	$l \cdot \mu\text{mol}^{-1} \cdot s^{-1}$	<input checked="" type="checkbox"/>

6 Rule

This is an overview of one rule.

6.1 Rule FeIII_t

Rule FeIII_t is an assignment rule for species FeIII_t:

$$\text{FeIII}_t = [\text{FeIII}] + [\text{FeIII_star}] \quad (1)$$

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

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

Nº	Id	Name	Reaction Equation	SBO
1	r1		$\text{FeIII} + \text{NADPH} \longrightarrow \text{FeII} + \text{NADPplus}$	0000200
2	r2		$\text{FeII} + \text{O2} \longrightarrow \text{FeII_O2}$	0000177
3	r3		$\text{FeII_O2} \longrightarrow \text{FeIII_star}$	0000201
4	r4		$\text{FeIII_star} + 0 \cdot 5 \text{ NADPH} \longrightarrow \text{FeII_star} + 0 \cdot 5 \text{ NADPplus}$	0000200
5	r5		$\text{FeII_star} + \text{O2} \longrightarrow \text{FeII_star_O2}$	0000177
6	r6		$\text{FeII_star_O2} \longrightarrow \text{FeIII_NO} + \text{citrulline}$	0000182
7	rF		$\text{FeIII_NO} \longrightarrow \text{FeIII} + \text{NO}$	0000180
8	rG		$\text{FeIII_NO} + 0 \cdot 5 \text{ NADPH} \longrightarrow \text{FeII_NO} + 0 \cdot 5 \text{ NADPplus}$	0000200
9	r9		$\text{FeII_NO} \longrightarrow \text{FeII} + \text{NO}$	0000180
10	r10		$\text{FeII_NO} + \text{O2} \longrightarrow \text{FeIII} + \text{NO3}$	0000200

7.1 Reaction r1

This is an irreversible reaction of two reactants forming two products.

SBO:0000200 redox reaction

Reaction equation



Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
FeIII	FeIII	
NADPH	NADPH	

Products

Table 7: Properties of each product.

Id	Name	SBO
FeII	FeII	
NADPplus	NADPplus	

Kinetic Law

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

$$v_1 = \text{vol}(\text{cytosol}) \cdot k_1 \cdot [\text{FeIII}] \quad (3)$$

7.2 Reaction r2

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

SBO:0000177 non-covalent binding

Reaction equation



Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
FeII	FeII	
O2	O2	

Product

Table 9: Properties of each product.

Id	Name	SBO
FeII_O2	FeII_O2	

Kinetic Law

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

$$v_2 = \text{vol}(\text{cytosol}) \cdot k_2 \cdot [\text{FeII}] \cdot [\text{O2}] \quad (5)$$

7.3 Reaction r3

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

SBO:0000201 oxidation

Reaction equation



Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
FeII_O2	FeII_O2	

Product

Table 11: Properties of each product.

Id	Name	SBO
FeIII_star	FeIII_star	

Id	Name	SBO
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Kinetic Law

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

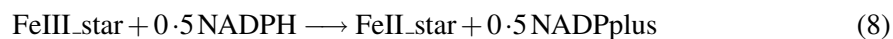
$$v_3 = \text{vol}(\text{cytosol}) \cdot k_3 \cdot [\text{FeII_O2}] \quad (7)$$

7.4 Reaction r4

This is an irreversible reaction of two reactants forming two products.

SBO:0000200 redox reaction

Reaction equation



Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
FeIII_star	FeIII_star	
NADPH	NADPH	

Products

Table 13: Properties of each product.

Id	Name	SBO
FeII_star	FeII_star	
NADPplus	NADPplus	

Kinetic Law

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

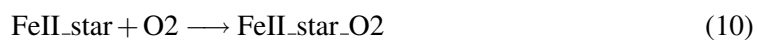
$$v_4 = \text{vol}(\text{cytosol}) \cdot k_4 \cdot [\text{FeIII_star}] \quad (9)$$

7.5 Reaction r5

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

SBO:0000177 non-covalent binding

Reaction equation



Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
FeII_star	FeII_star	
O2	O2	

Product

Table 15: Properties of each product.

Id	Name	SBO
FeII_star_O2	FeII_star_O2	

Kinetic Law

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

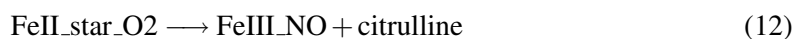
$$v_5 = \text{vol}(\text{cytosol}) \cdot k_5 \cdot [\text{FeII_star}] \cdot [\text{O2}] \quad (11)$$

7.6 Reaction r6

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

SBO:0000182 conversion

Reaction equation



Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
FeII_star_O2	FeII_star_O2	

Products

Table 17: Properties of each product.

Id	Name	SBO
FeIII_NO	FeIII_NO	
citrulline	citruline	

Kinetic Law

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

$$v_6 = \text{vol}(\text{cytosol}) \cdot k_6 \cdot [\text{FeII_star_O2}] \quad (13)$$

7.7 Reaction rF

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

SBO:0000180 dissociation

Reaction equation



Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
FeIII_NO	FeIII_NO	

Products

Table 19: Properties of each product.

Id	Name	SBO
FeIII	FeIII	

Id	Name	SBO
NO	NO	

Kinetic Law

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

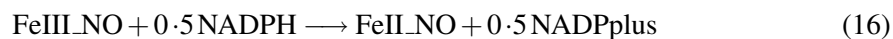
$$v_7 = \text{vol}(\text{cytosol}) \cdot k_7 \cdot [\text{FeIII_NO}] \quad (15)$$

7.8 Reaction rG

This is an irreversible reaction of two reactants forming two products.

SBO:0000200 redox reaction

Reaction equation



Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
FeIII_NO	FeIII_NO	
NADPH	NADPH	

Products

Table 21: Properties of each product.

Id	Name	SBO
FeII_NO	FeII_NO	
NADPplus	NADPplus	

Kinetic Law

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

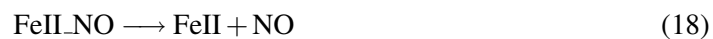
$$v_8 = \text{vol}(\text{cytosol}) \cdot k_8 \cdot [\text{FeIII_NO}] \quad (17)$$

7.9 Reaction r9

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

SBO:0000180 dissociation

Reaction equation



Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
FeII_NO	FeII_NO	

Products

Table 23: Properties of each product.

Id	Name	SBO
FeII	FeII	
NO	NO	

Kinetic Law

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

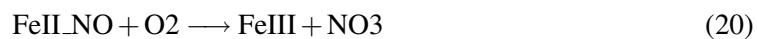
$$v_9 = \text{vol}(\text{cytosol}) \cdot k_9 \cdot [\text{FeII_NO}] \quad (19)$$

7.10 Reaction r10

This is an irreversible reaction of two reactants forming two products.

SBO:0000200 redox reaction

Reaction equation



Reactants

Table 24: Properties of each reactant.

Id	Name	SBO
FeII_NO O2	FeII_NO O2	

Products

Table 25: Properties of each product.

Id	Name	SBO
FeIII NO3	FeIII NO3	

Kinetic Law

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

$$v_{10} = \text{vol}(\text{cytosol}) \cdot k_{10} \cdot [\text{FeII_NO}] \cdot [\text{O2}] \quad (21)$$

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.

8.1 Species FeIII

Name FeIII

SBO:0000297 protein complex

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

This species takes part in three reactions (as a reactant in [r1](#) and as a product in [rF](#), [r10](#)).

$$\frac{d}{dt}\text{FeIII} = v_7 + v_{10} - v_1 \quad (22)$$

8.2 Species FeII

Name FeII

SBO:0000297 protein complex

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

This species takes part in three reactions (as a reactant in [r2](#) and as a product in [r1](#), [r9](#)).

$$\frac{d}{dt}\text{FeII} = v_1 + v_9 - v_2 \quad (23)$$

8.3 Species [FeII_O2](#)

Name FeII_O2

SBO:0000297 protein complex

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

This species takes part in two reactions (as a reactant in [r3](#) and as a product in [r2](#)).

$$\frac{d}{dt}\text{FeII_O2} = v_2 - v_3 \quad (24)$$

8.4 Species [FeIII_star](#)

Name FeIII_star

SBO:0000297 protein complex

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

This species takes part in two reactions (as a reactant in [r4](#) and as a product in [r3](#)).

$$\frac{d}{dt}\text{FeIII_star} = v_3 - v_4 \quad (25)$$

8.5 Species [FeII_star](#)

Name FeII_star

SBO:0000297 protein complex

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

This species takes part in two reactions (as a reactant in [r5](#) and as a product in [r4](#)).

$$\frac{d}{dt}\text{FeII_star} = v_4 - v_5 \quad (26)$$

8.6 Species [FeII_star_O2](#)

Name FeII_star_O2

SBO:0000297 protein complex

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

This species takes part in two reactions (as a reactant in [r6](#) and as a product in [r5](#)).

$$\frac{d}{dt}\text{FeII_star_O2} = v_5 - v_6 \quad (27)$$

8.7 Species FeIII_NO

Name FeIII_NO

SBO:0000297 protein complex

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

This species takes part in three reactions (as a reactant in [rF](#), [rG](#) and as a product in [r6](#)).

$$\frac{d}{dt}\text{FeIII_NO} = v_6 - v_7 - v_8 \quad (28)$$

8.8 Species FeII_NO

Name FeII_NO

SBO:0000297 protein complex

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

This species takes part in three reactions (as a reactant in [r9](#), [r10](#) and as a product in [rG](#)).

$$\frac{d}{dt}\text{FeII_NO} = v_8 - v_9 - v_{10} \quad (29)$$

8.9 Species NADPH

Name NADPH

SBO:0000247 simple chemical

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

This species takes part in three reactions (as a reactant in [r1](#), [r4](#), [rG](#)), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{NADPH} = 0 \quad (30)$$

8.10 Species O_2

Name O_2

SBO:0000247 simple chemical

Initial concentration $140 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [r2](#), [r5](#), [r10](#)), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{O}_2 = 0 \quad (31)$$

8.11 Species citrulline

Name citrulline

SBO:0000247 simple chemical

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

This species takes part in one reaction (as a product in [r6](#)), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{citrulline} = 0 \quad (32)$$

8.12 Species NO3

Name NO3

SBO:0000247 simple chemical

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

This species takes part in one reaction (as a product in [r10](#)), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{NO3} = 0 \quad (33)$$

8.13 Species NO

Name NO

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a product in [rF](#), [r9](#)), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{NO} = 0 \quad (34)$$

8.14 Species NADPplus

Name NADPplus

SBO:0000327 non-macromolecular ion

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

This species takes part in three reactions (as a product in [r1](#), [r4](#), [rG](#)), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{NADPplus} = 0 \quad (35)$$

8.15 Species `FeIII_t`

Name `FeIII_t`

SBO:0000297 protein complex

Involved in rule `FeIII_t`

One rule which determines this species' quantity.

A Glossary of Systems Biology Ontology Terms

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:0000177 non-covalent binding: Interaction between several biochemical entities that results in the formation of a non-covalent complex

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

SBO:0000182 conversion: Biochemical reaction that results in the modification of some covalent bonds

SBO:0000200 redox reaction: Chemical process in which atoms have their oxidation number (oxidation state) changed

SBO:0000201 oxidation: Chemical process during which a molecular entity loses electrons

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

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

SBO:0000327 non-macromolecular ion: Chemical entity having a net electric charge

SBO:0000339 bimolecular association rate constant: Rate with which two components associate into a complex

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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