

## SBML Model Report

**Model name: “Zi2007\_TGFbeta\_signaling”**



May 5, 2016

### 1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following three authors: Harish Dharuri<sup>1</sup>, Edda Klipp<sup>2</sup> and Kun Yang<sup>3</sup> at February 14<sup>th</sup> 2008 at 9:21 a. m. and last time modified at July fifth 2012 at 4:45 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	3
species types	0	species	16
events	0	constraints	0
reactions	26	function definitions	0
global parameters	20	unit definitions	2
rules	2	initial assignments	0

### Model Notes

The model reproduces the time profiles of Total Smad2 in the nucleus as well as the cytoplasm as depicted in 2D and also the other time profiles as depicted in Fig 2. Two parameters that are not present in the paper are introduced here for illustration purposes and they are Total Smad2n and Total Smad2c. The term  $kr_{EE*LRC_{EE}}$  has not been included in the ODE's for T1R\_surf,

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T2R\_surf and TGFbeta in the paper but is included in this model. MathSBML was used to reproduce the simulation result.

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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** minute

**Definition** 60 s

### 2.2 Unit substance

**Name** nano mole

**Definition** nmol

### 2.3 Unit volume

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

**Definition** l

### 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 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
V_medium	Medium		3	1	litre	✓	
V_nuc	Nucleus		3	$3.5 \cdot 10^{-4}$	l	✓	V_cyt
V_cyt	Cytoplasm		3	0.00105	l	✓	V_medium

### 3.1 Compartment V\_medium

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

**Name** Medium

### 3.2 Compartment V\_nuc

This is a three dimensional compartment with a constant size of  $3.5 \cdot 10^{-4}$  litre, which is surrounded by V\_cyt (Cytoplasm).

**Name** Nucleus

### 3.3 Compartment V\_cyt

This is a three dimensional compartment with a constant size of 0.00105 litre, which is surrounded by V\_medium (Medium).

**Name** Cytoplasm

## 4 Species

This model contains 16 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
Smad2c	Smad2c	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
Smad2n	Smad2n	V_nuc	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
Smad4c	Smad4c	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
Smad4n	Smad4n	V_nuc	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
T1R_Surf	T1R_Surf	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
T1R_Cave	T1R_Cave	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
T1R_EE	T1R_EE	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
T2R_Surf	T2R_Surf	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
T2R_Cave	T2R_Cave	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
T2R_EE	T2R_EE	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
LRC_Surf	LRC_Surf	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
LRC_Cave	LRC_Cave	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
LRC_EE	LRC_EE	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
Smads_Complex_c	Smads_Complex_c	V_cyt	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
Smads_Complex_n	Smads_Complex_n	V_nuc	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$
TGF_beta	TGF_beta	V_medium	$\text{nmol} \cdot \text{l}^{-1}$	$\square$	$\square$

## 5 Parameters

This model contains 20 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v_T1R			0.010		<input checked="" type="checkbox"/>
v_T2R			0.029		<input checked="" type="checkbox"/>
ki_EE			0.330		<input checked="" type="checkbox"/>
kr_EE			0.033		<input checked="" type="checkbox"/>
ki_Cave			0.330		<input checked="" type="checkbox"/>
kr_Cave			0.037		<input checked="" type="checkbox"/>
Kcd			0.005		<input checked="" type="checkbox"/>
k_LRC			2197.000		<input type="checkbox"/>
Klid			0.026		<input checked="" type="checkbox"/>
Kdeg_T1R_EE			0.005		<input checked="" type="checkbox"/>
Kdeg_T2R_EE			0.025		<input checked="" type="checkbox"/>
Kimp_Smad2c			0.160		<input checked="" type="checkbox"/>
Kexp_Smad2n			1.000		<input checked="" type="checkbox"/>
Kimp_Smad4c			0.080		<input checked="" type="checkbox"/>
Kexp_Smad4n			0.500		<input checked="" type="checkbox"/>
k_Smads- _Complex_c			$6.85 \cdot 10^{-5}$		<input checked="" type="checkbox"/>
Kimp_Smads- _Complex_c			0.160		<input checked="" type="checkbox"/>
Kdiss_Smads- _Complex_n			0.117		<input checked="" type="checkbox"/>
Total_Smad2n			0.000		<input type="checkbox"/>
Total_Smad2c			0.000		<input type="checkbox"/>

## 6 Rules

This is an overview of two rules.

### 6.1 Rule Total\_Smad2n

Rule Total\_Smad2n is an assignment rule for parameter Total\_Smad2n:

$$\text{Total\_Smad2n} = [\text{Smad2n}] + [\text{Smads\_Complex\_n}] \quad (1)$$

**Derived unit**  $\text{nmol} \cdot \text{l}^{-1}$

## 6.2 Rule `Total_Smad2c`

Rule `Total_Smad2c` is an assignment rule for parameter `Total_Smad2c`:

$$\text{Total\_Smad2c} = [\text{Smad2c}] + [\text{Smads\_Complex\_c}] \quad (2)$$

**Derived unit**  $\text{nmol} \cdot \text{l}^{-1}$

## 7 Reactions

This model contains 26 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_Smad2_import		$\text{Smad2c} \longrightarrow \text{Smad2n}$	
2	R2_Smad2_export		$\text{Smad2n} \longrightarrow \text{Smad2c}$	
3	R3_Smad4_import		$\text{Smad4c} \longrightarrow \text{Smad4n}$	
4	R4_Smad4_export		$\text{Smad4n} \longrightarrow \text{Smad4c}$	
5	R5_T1R- _production		$\emptyset \longrightarrow \text{T1R\_Surf}$	
6	R6_T1R_Cave- _formation		$\text{T1R\_Surf} \longrightarrow \text{T1R\_Cave}$	
7	R7_T1R_Cave- _recycling		$\text{T1R\_Cave} \longrightarrow \text{T1R\_Surf}$	
8	R8_T1R_EE- _formation		$\text{T1R\_Surf} \longrightarrow \text{T1R\_EE}$	
9	R9_T1R_EE- _recycling		$\text{T1R\_EE} \longrightarrow \text{T1R\_Surf}$	
10	R10_T1R_EE- _degradation		$\text{T1R\_EE} \longrightarrow \emptyset$	
11	R11_T2R- _production		$\emptyset \longrightarrow \text{T2R\_Surf}$	
12	R12_T2R_Cave- _formation		$\text{T2R\_Surf} \longrightarrow \text{T2R\_Cave}$	
13	R13_T2R_Cave- _recycling		$\text{T2R\_Cave} \longrightarrow \text{T2R\_Surf}$	

Nº	Id	Name	Reaction Equation	SBO
14	R14.T2R_EE- _formation		$T2R\_Surf \longrightarrow T2R\_EE$	
15	R15.T2R_EE- _recycling		$T2R\_EE \longrightarrow T2R\_Surf + TGF\_beta$	
16	R16.T2R_EE- _degradation		$T2R\_EE \longrightarrow \emptyset$	
17	R17.LRC- _formation		$TGF\_beta + T2R\_Surf + T1R\_Surf \longrightarrow LRC\_Surf$	
18	R18.LRC_Cave- _formation		$LRC\_Surf \longrightarrow LRC\_Cave$	
19	R19.LRC_Cave- _recycling		$LRC\_Cave \longrightarrow T1R\_Surf + TGF\_beta + T2R\_Surf$	
20	R20.LRC_EE- _formation		$LRC\_Surf \longrightarrow LRC\_EE$	
21	R21.LRC_EE- _recycling		$LRC\_EE \longrightarrow T1R\_Surf + T2R\_Surf + TGF\_beta$	
22	R22.LRC_EE- _degradation		$LRC\_EE \longrightarrow \emptyset$	
23	R23.Smads- _Complex- _formation		$Smad2c + Smad4c \xrightarrow{LRC\_EE} Smads\_Complex\_c$	
24	R24.Smads- _Complex_import		$Smads\_Complex\_c \longrightarrow Smads\_Complex\_n$	
25	R25.Smads- _Complex- _Dissociation		$Smads\_Complex\_n \longrightarrow Smad4n + Smad2n$	
26	R26.LRC_Cave- _degradation		$LRC\_Cave \xrightarrow{Smads\_Complex\_n} \emptyset$	



## 7.1 Reaction R1\_Smad2\_import

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

### Reaction equation



### Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
Smad2c	Smad2c	

### Product

Table 7: Properties of each product.

Id	Name	SBO
Smad2n	Smad2n	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_1 = \text{vol}(\text{V\_cyt}) \cdot \text{Kimp\_Smad2c} \cdot [\text{Smad2c}] \quad (4)$$

## 7.2 Reaction R2\_Smad2\_export

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

### Reaction equation



### Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Smad2n	Smad2n	

## Product

Table 9: Properties of each product.

Id	Name	SBO
Smad2c	Smad2c	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_2 = \text{vol}(\text{V\_nuc}) \cdot \text{Kexp\_Smad2n} \cdot [\text{Smad2n}] \quad (6)$$

## 7.3 Reaction R3\_Smad4\_import

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

## Reaction equation



## Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
Smad4c	Smad4c	

## Product

Table 11: Properties of each product.

Id	Name	SBO
Smad4n	Smad4n	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_3 = \text{vol}(\text{V\_cyt}) \cdot \text{Kimp\_Smad4c} \cdot [\text{Smad4c}] \quad (8)$$

## 7.4 Reaction R4\_Smad4\_export

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

### Reaction equation



### Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Smad4n	Smad4n	

### Product

Table 13: Properties of each product.

Id	Name	SBO
Smad4c	Smad4c	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_4 = \text{vol}(\text{V\_nuc}) \cdot K_{\text{exp\_Smad4n}} \cdot [\text{Smad4n}] \quad (10)$$

## 7.5 Reaction R5\_T1R\_production

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

### Reaction equation



### Product

Table 14: Properties of each product.

Id	Name	SBO
T1R_Surf	T1R_Surf	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_5 = \text{vol}(\text{V\_cyt}) \cdot v_{\text{T1R}} \quad (12)$$

## 7.6 Reaction R6\_T1R\_Cave\_formation

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

### Reaction equation



### Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
T1R_Surf	T1R_Surf	

### Product

Table 16: Properties of each product.

Id	Name	SBO
T1R_Cave	T1R_Cave	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_6 = \text{vol}(\text{V\_cyt}) \cdot k_{\text{i\_Cave}} \cdot [\text{T1R\_Surf}] \quad (14)$$

## 7.7 Reaction R7\_T1R\_Cave\_recycling

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

### Reaction equation



### Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
T1R_Cave	T1R_Cave	

## Product

Table 18: Properties of each product.

Id	Name	SBO
T1R_Surf	T1R_Surf	

## Kinetic Law

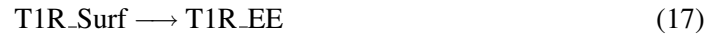
**Derived unit** contains undeclared units

$$v_7 = \text{vol}(\text{V\_cyt}) \cdot \text{kr\_Cave} \cdot [\text{T1R\_Cave}] \quad (16)$$

## 7.8 Reaction R8\_T1R\_EE\_formation

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

## Reaction equation



## Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
T1R_Surf	T1R_Surf	

## Product

Table 20: Properties of each product.

Id	Name	SBO
T1R_EE	T1R_EE	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_8 = \text{vol}(\text{V\_cyt}) \cdot k_{i\_EE} \cdot [\text{T1R\_Surf}] \quad (18)$$

## 7.9 Reaction `R9_T1R_EE_recycling`

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

### Reaction equation



### Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
T1R_EE	T1R_EE	

### Product

Table 22: Properties of each product.

Id	Name	SBO
T1R_Surf	T1R_Surf	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_9 = \text{vol}(\text{V\_cyt}) \cdot k_{r\_EE} \cdot [\text{T1R\_EE}] \quad (20)$$

## 7.10 Reaction `R10_T1R_EE_degradation`

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

### Reaction equation



### Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
T1R_EE	T1R_EE	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{10} = \text{vol}(\text{V\_cyt}) \cdot \text{Kdeg\_T1R\_EE} \cdot [\text{T1R\_EE}] \quad (22)$$

### 7.11 Reaction R11\_T2R\_production

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

#### Reaction equation



### Product

Table 24: Properties of each product.

Id	Name	SBO
T2R_Surf	T2R_Surf	

### Kinetic Law

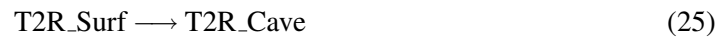
**Derived unit** contains undeclared units

$$v_{11} = \text{vol}(\text{V\_cyt}) \cdot v_{\text{T2R}} \quad (24)$$

### 7.12 Reaction R12\_T2R\_Cave\_formation

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

#### Reaction equation



### Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
T2R_Surf	T2R_Surf	

## Product

Table 26: Properties of each product.

Id	Name	SBO
T2R_Cave	T2R_Cave	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{12} = \text{vol}(\text{V\_cyt}) \cdot k_{\text{i\_Cave}} \cdot [\text{T2R\_Surf}] \quad (26)$$

### 7.13 Reaction [R13\\_T2R\\_Cave\\_recycling](#)

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

## Reaction equation



## Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
T2R_Cave	T2R_Cave	

## Product

Table 28: Properties of each product.

Id	Name	SBO
T2R_Surf	T2R_Surf	



## Kinetic Law

**Derived unit** contains undeclared units

$$v_{13} = \text{vol}(\text{V\_cyt}) \cdot \text{kr\_Cave} \cdot [\text{T2R\_Cave}] \quad (28)$$

## 7.14 Reaction R14\_T2R\_EE\_formation

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

### Reaction equation



### Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
T2R_Surf	T2R_Surf	

### Product

Table 30: Properties of each product.

Id	Name	SBO
T2R_EE	T2R_EE	

## Kinetic Law

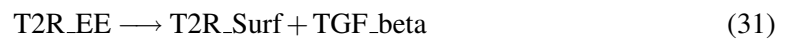
**Derived unit** contains undeclared units

$$v_{14} = \text{vol}(\text{V\_cyt}) \cdot \text{ki\_EE} \cdot [\text{T2R\_Surf}] \quad (30)$$

## 7.15 Reaction R15\_T2R\_EE\_recycling

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

### Reaction equation



### Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
T2R_EE	T2R_EE	

## Products

Table 32: Properties of each product.

Id	Name	SBO
T2R_Surf	T2R_Surf	
TGF_beta	TGF_beta	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{15} = \text{vol}(V_{\text{cyt}}) \cdot k_{\text{r\_EE}} \cdot [\text{T2R\_EE}] \quad (32)$$

### 7.16 Reaction R16\_T2R\_EE\_degradation

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

#### Reaction equation



## Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
T2R_EE	T2R_EE	

## Kinetic Law

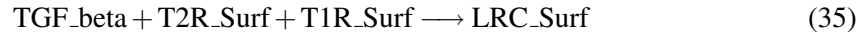
**Derived unit** contains undeclared units

$$v_{16} = \text{vol}(V_{\text{cyt}}) \cdot K_{\text{deg\_T2R\_EE}} \cdot [\text{T2R\_EE}] \quad (34)$$

### 7.17 Reaction R17\_LRC\_formation

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

### Reaction equation



### Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
TGF_beta	TGF_beta	
T2R_Surf	T2R_Surf	
T1R_Surf	T1R_Surf	

### Product

Table 35: Properties of each product.

Id	Name	SBO
LRC_Surf	LRC_Surf	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{17} = \text{vol}(\text{V\_cyt}) \cdot k_{\text{LRC}} \cdot [\text{TGF\_beta}] \cdot [\text{T2R\_Surf}] \cdot [\text{T1R\_Surf}] \quad (36)$$

### 7.18 Reaction R18\_LRC\_Cave\_formation

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

### Reaction equation



### Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
LRC_Surf	LRC_Surf	

## Product

Table 37: Properties of each product.

Id	Name	SBO
LRC_Cave	LRC_Cave	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{18} = \text{vol}(V_{\text{cyt}}) \cdot k_{\text{i\_Cave}} \cdot [\text{LRC\_Surf}] \quad (38)$$

## 7.19 Reaction R19\_LRC\_Cave\_recycling

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

## Reaction equation



## Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
LRC_Cave	LRC_Cave	

## Products

Table 39: Properties of each product.

Id	Name	SBO
T1R_Surf	T1R_Surf	
TGF_beta	TGF_beta	
T2R_Surf	T2R_Surf	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{19} = \text{vol}(V_{\text{cyt}}) \cdot k_{\text{r\_Cave}} \cdot [\text{LRC\_Cave}] \quad (40)$$

## 7.20 Reaction R20\_LRC\_EE\_formation

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

### Reaction equation



### Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
LRC_Surf	LRC_Surf	

### Product

Table 41: Properties of each product.

Id	Name	SBO
LRC_EE	LRC_EE	

### Kinetic Law

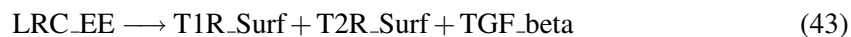
**Derived unit** contains undeclared units

$$v_{20} = \text{vol}(\text{V\_cyt}) \cdot k_{i\_EE} \cdot [\text{LRC\_Surf}] \quad (42)$$

## 7.21 Reaction R21\_LRC\_EE\_recycling

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

### Reaction equation



### Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
LRC_EE	LRC_EE	

## Products

Table 43: Properties of each product.

Id	Name	SBO
T1R_Surf	T1R_Surf	
T2R_Surf	T2R_Surf	
TGF_beta	TGF_beta	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{21} = \text{vol}(V_{\text{cyt}}) \cdot \text{kr\_EE} \cdot [\text{LRC\_EE}] \quad (44)$$

### 7.22 Reaction R22\_LRC\_EE\_degradation

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

## Reaction equation



## Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
LRC_EE	LRC_EE	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{22} = \text{vol}(V_{\text{cyt}}) \cdot \text{Kcd} \cdot [\text{LRC\_EE}] \quad (46)$$

### 7.23 Reaction R23\_Smads\_Complex\_formation

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

## Reaction equation



## Reactants

Table 45: Properties of each reactant.

Id	Name	SBO
Smad2c	Smad2c	
Smad4c	Smad4c	

## Modifier

Table 46: Properties of each modifier.

Id	Name	SBO
LRC_EE	LRC_EE	

## Product

Table 47: Properties of each product.

Id	Name	SBO
Smads_Complex_c	Smads_Complex_c	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{23} = \text{vol}(\text{V\_cyt}) \cdot k\_Smads\_Complex\_c \cdot [\text{Smad2c}] \cdot [\text{Smad4c}] \cdot [\text{LRC\_EE}] \quad (48)$$

### 7.24 Reaction `R24_Smads_Complex_import`

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

#### Reaction equation



## Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
Smads_Complex_c	Smads_Complex_c	

## Product

Table 49: Properties of each product.

Id	Name	SBO
Smads_Complex_n	Smads_Complex_n	

## Kinetic Law

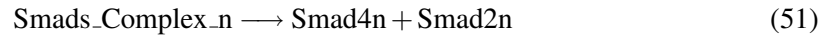
**Derived unit** contains undeclared units

$$v_{24} = \text{vol}(\text{V\_cyt}) \cdot \text{Kimp\_Smads\_Complex\_c} \cdot [\text{Smads\_Complex\_c}] \quad (50)$$

## 7.25 Reaction R25\_Smads\_Complex\_Dissociation

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

## Reaction equation



## Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
Smads_Complex_n	Smads_Complex_n	

## Products

Table 51: Properties of each product.

Id	Name	SBO
Smad4n	Smad4n	
Smad2n	Smad2n	



## Kinetic Law

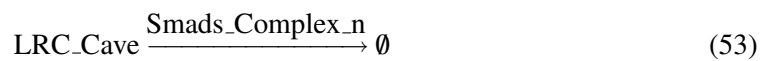
**Derived unit** contains undeclared units

$$v_{25} = \text{vol}(V_{\text{nuc}}) \cdot K_{\text{diss\_Smads\_Complex\_n}} \cdot [\text{Smads\_Complex\_n}] \quad (52)$$

## 7.26 Reaction R26\_LRC\_Cave\_degradation

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

### Reaction equation



### Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
LRC_Cave	LRC_Cave	

### Modifier

Table 53: Properties of each modifier.

Id	Name	SBO
Smads_Complex_n	Smads_Complex_n	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{26} = \text{vol}(V_{\text{cyt}}) \cdot K_{\text{id}} \cdot [\text{LRC\_Cave}] \cdot [\text{Smads\_Complex\_n}] \quad (54)$$

## 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 `Smad2c`

**Name** `Smad2c`

**Initial concentration**  $492.61 \text{ nmol} \cdot \text{l}^{-1}$

**Charge** 0

This species takes part in three reactions (as a reactant in `R1_Smad2_import`, `R23_Smads_Complex_formation` and as a product in `R2_Smad2_export`).

$$\frac{d}{dt}\text{Smad2c} = v_2 - v_1 - v_{23} \quad (55)$$

### 8.2 Species `Smad2n`

**Name** `Smad2n`

**Initial concentration**  $236.45 \text{ nmol} \cdot \text{l}^{-1}$

**Charge** 0

This species takes part in three reactions (as a reactant in `R2_Smad2_export` and as a product in `R1_Smad2_import`, `R25_Smads_Complex_Dissociation`).

$$\frac{d}{dt}\text{Smad2n} = v_1 + v_{25} - v_2 \quad (56)$$

### 8.3 Species `Smad4c`

**Name** `Smad4c`

**Initial concentration**  $1149.4 \text{ nmol} \cdot \text{l}^{-1}$

**Charge** 0

This species takes part in three reactions (as a reactant in `R3_Smad4_import`, `R23_Smads_Complex_formation` and as a product in `R4_Smad4_export`).

$$\frac{d}{dt}\text{Smad4c} = v_4 - v_3 - v_{23} \quad (57)$$

## 8.4 Species Smad4n

**Name** Smad4n

**Initial concentration** 551.72 nmol · l<sup>-1</sup>

**Charge** 0

This species takes part in three reactions (as a reactant in [R4\\_Smad4\\_export](#) and as a product in [R3\\_Smad4\\_import](#), [R25\\_Smads\\_Complex\\_Dissociation](#)).

$$\frac{d}{dt}\text{Smad4n} = v_3 + v_{25} - v_4 \quad (58)$$

## 8.5 Species T1R\_Surf

**Name** T1R\_Surf

**Initial concentration** 0.237 nmol · l<sup>-1</sup>

**Charge** 0

This species takes part in eight reactions (as a reactant in [R6\\_T1R\\_Cave\\_formation](#), [R8\\_T1R\\_EE\\_formation](#), [R17\\_LRC\\_formation](#) and as a product in [R5\\_T1R\\_production](#), [R7\\_T1R\\_Cave\\_recycling](#), [R9\\_T1R\\_EE\\_recycling](#), [R19\\_LRC\\_Cave\\_recycling](#), [R21\\_LRC\\_EE\\_recycling](#)).

$$\frac{d}{dt}\text{T1R_Surf} = v_5 + v_7 + v_9 + v_{19} + v_{21} - v_6 - v_8 - v_{17} \quad (59)$$

## 8.6 Species T1R\_Cave

**Name** T1R\_Cave

**Initial concentration** 2.092 nmol · l<sup>-1</sup>

**Charge** 0

This species takes part in two reactions (as a reactant in [R7\\_T1R\\_Cave\\_recycling](#) and as a product in [R6\\_T1R\\_Cave\\_formation](#)).

$$\frac{d}{dt}\text{T1R_Cave} = v_6 - v_7 \quad (60)$$

## 8.7 Species T1R\_EE

**Name** T1R\_EE

**Initial concentration**  $2.06 \text{ nmol} \cdot \text{l}^{-1}$

**Charge** 0

This species takes part in three reactions (as a reactant in [R9\\_T1R\\_EE\\_recycling](#), [R10\\_T1R\\_EE\\_degradation](#) and as a product in [R8\\_T1R\\_EE\\_formation](#)).

$$\frac{d}{dt} \text{T1R\_EE} = v_8 - v_9 - v_{10} \quad (61)$$

## 8.8 Species T2R\_Surf

**Name** T2R\_Surf

**Initial concentration**  $0.202 \text{ nmol} \cdot \text{l}^{-1}$

**Charge** 0

This species takes part in eight reactions (as a reactant in [R12\\_T2R\\_Cave\\_formation](#), [R14\\_T2R\\_EE\\_formation](#), [R17\\_LRC\\_formation](#) and as a product in [R11\\_T2R\\_production](#), [R13\\_T2R\\_Cave\\_recycling](#), [R15\\_T2R\\_EE\\_recycling](#), [R19\\_LRC\\_Cave\\_recycling](#), [R21\\_LRC\\_EE\\_recycling](#)).

$$\frac{d}{dt} \text{T2R\_Surf} = v_{11} + v_{13} + v_{15} + v_{19} + v_{21} - v_{12} - v_{14} - v_{17} \quad (62)$$

## 8.9 Species T2R\_Cave

**Name** T2R\_Cave

**Initial concentration**  $1.778 \text{ nmol} \cdot \text{l}^{-1}$

**Charge** 0

This species takes part in two reactions (as a reactant in [R13\\_T2R\\_Cave\\_recycling](#) and as a product in [R12\\_T2R\\_Cave\\_formation](#)).

$$\frac{d}{dt} \text{T2R\_Cave} = v_{12} - v_{13} \quad (63)$$

### 8.10 Species T2R\_EE

**Name** T2R\_EE

**Initial concentration** 1.148 nmol · l<sup>-1</sup>

**Charge** 0

This species takes part in three reactions (as a reactant in [R15\\_T2R\\_EE\\_recycling](#), [R16\\_T2R\\_EE\\_degradation](#) and as a product in [R14\\_T2R\\_EE\\_formation](#)).

$$\frac{d}{dt} \text{T2R\_EE} = v_{14} - v_{15} - v_{16} \quad (64)$$

### 8.11 Species LRC\_Surf

**Name** LRC\_Surf

**Initial concentration** 0 nmol · l<sup>-1</sup>

**Charge** 0

This species takes part in three reactions (as a reactant in [R18\\_LRC\\_Cave\\_formation](#), [R20\\_LRC\\_EE\\_formation](#) and as a product in [R17\\_LRC\\_formation](#)).

$$\frac{d}{dt} \text{LRC\_Surf} = v_{17} - v_{18} - v_{20} \quad (65)$$

### 8.12 Species LRC\_Cave

**Name** LRC\_Cave

**Initial concentration** 0 nmol · l<sup>-1</sup>

**Charge** 0

This species takes part in three reactions (as a reactant in [R19\\_LRC\\_Cave\\_recycling](#), [R26\\_LRC\\_Cave\\_degradation](#) and as a product in [R18\\_LRC\\_Cave\\_formation](#)).

$$\frac{d}{dt} \text{LRC\_Cave} = v_{18} - v_{19} - v_{26} \quad (66)$$

### 8.13 Species LRC\_EE

**Name** LRC\_EE

**Initial concentration** 0 nmol · l<sup>-1</sup>

**Charge** 0

This species takes part in four reactions (as a reactant in [R21\\_LRC\\_EE\\_recycling](#), [R22\\_LRC\\_EE\\_degradation](#) and as a product in [R20\\_LRC\\_EE\\_formation](#) and as a modifier in [R23\\_Smads\\_Complex\\_formation](#)).

$$\frac{d}{dt}\text{LRC\_EE} = v_{20} - v_{21} - v_{22} \quad (67)$$

#### 8.14 Species [Smads\\_Complex\\_c](#)

**Name** Smads\_Complex\_c

**Initial concentration** 0 nmol · l<sup>-1</sup>

**Charge** 0

This species takes part in two reactions (as a reactant in [R24\\_Smads\\_Complex\\_import](#) and as a product in [R23\\_Smads\\_Complex\\_formation](#)).

$$\frac{d}{dt}\text{Smads\_Complex\_c} = v_{23} - v_{24} \quad (68)$$

#### 8.15 Species [Smads\\_Complex\\_n](#)

**Name** Smads\_Complex\_n

**Initial concentration** 0 nmol · l<sup>-1</sup>

**Charge** 0

This species takes part in three reactions (as a reactant in [R25\\_Smads\\_Complex\\_Dissociation](#) and as a product in [R24\\_Smads\\_Complex\\_import](#) and as a modifier in [R26\\_LRC\\_Cave\\_degradation](#)).

$$\frac{d}{dt}\text{Smads\_Complex\_n} = v_{24} - v_{25} \quad (69)$$

#### 8.16 Species [TGF\\_beta](#)

**Name** TGF\_beta

**Initial concentration** 0.08 nmol · l<sup>-1</sup>

**Charge** 0

This species takes part in four reactions (as a reactant in [R17\\_LRC\\_formation](#) and as a product in [R15\\_T2R\\_EE\\_recycling](#), [R19\\_LRC\\_Cave\\_recycling](#), [R21\\_LRC\\_EE\\_recycling](#)).

$$\frac{d}{dt}\text{TGF\_beta} = v_{15} + v_{19} + v_{21} - v_{17} \quad (70)$$

SBML<sup>2</sup>TeX 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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