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[1], Edda Klipp[2] and Kun Yang[3] at February 14th 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.

To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

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^2

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	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Smad2n	Smad2n	V_nuc	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Smad4c	Smad4c	V_cyt	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Smad4n	Smad4n	V_nuc	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T1R_Surf	T1R_Surf	V_cyt	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T1R_Cave	T1R_Cave	V_cyt	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T1R_EE	T1R_EE	V_cyt	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T2R_Surf	T2R_Surf	V_cyt	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T2R_Cave	T2R_Cave	V_cyt	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T2R_EE	T2R_EE	V_cyt	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
LRC_Surf	LRC_Surf	V_cyt	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
LRC_Cave	LRC_Cave	V_cyt	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
LRC_EE	LRC_EE	V_cyt	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Smads_Complex_c	Smads_Complex_c	V_cyt	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Smads_Complex_n	Smads_Complex_n	V_nuc	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
TGF_beta	TGF_beta	V_medium	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 20 global parameters.

Table 4: Properties of each parameter.

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

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:

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

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

6.2 Rule Total_Smad2c

Rule Total_Smad2c is an assignment rule for parameter Total_Smad2c:

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

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

№	Id	Name	Reaction Equation	SBO
1	R1_Smad2_import		Smad2c ⟶ Smad2n	
2	R2_Smad2_export		Smad2n ⟶ Smad2c	
3	R3_Smad4_import		Smad4c ⟶ Smad4n	
4	R4_Smad4_export		Smad4n ⟶ Smad4c	
5	R5_T1R_production		∅ ⟶ T1R_Surf	
6	R6_T1R_Cave_formation		T1R_Surf ⟶ T1R_Cave	
7	R7_T1R_Cave_recycling		T1R_Cave ⟶ T1R_Surf	
8	R8_T1R_EE_formation		T1R_Surf ⟶ T1R_EE	
9	R9_T1R_EE_recycling		T1R_EE ⟶ T1R_Surf	
10	R10_T1R_EE_degradation		T1R_EE ⟶ ∅	
11	R11_T2R_production		∅ ⟶ T2R_Surf	
12	R12_T2R_Cave_formation		T2R_Surf ⟶ T2R_Cave	
13	R13_T2R_Cave_recycling		T2R_Cave ⟶ T2R_Surf	

№	Id	Name	Reaction Equation	SBO
14	R14_T2R_EE-_formation		$\text{T2R\_Surf} \longrightarrow \text{T2R\_EE}$	
15	R15_T2R_EE-_recycling		$\text{T2R\_EE} \longrightarrow \text{T2R\_Surf} + \text{TGF\_beta}$	
16	R16_T2R_EE-_degradation		$\text{T2R\_EE} \longrightarrow \emptyset$	
17	R17_LRC-_formation		$\text{TGF\_beta} + \text{T2R\_Surf} + \text{T1R\_Surf} \longrightarrow \text{LRC\_Surf}$	
18	R18_LRC_Cave-_formation		$\text{LRC\_Surf} \longrightarrow \text{LRC\_Cave}$	
19	R19_LRC_Cave-_recycling		$\text{LRC\_Cave} \longrightarrow \text{T1R\_Surf} + \text{TGF\_beta} + \text{T2R\_Surf}$	
20	R20_LRC_EE-_formation		$\text{LRC\_Surf} \longrightarrow \text{LRC\_EE}$	
21	R21_LRC_EE-_recycling		$\text{LRC\_EE} \longrightarrow \text{T1R\_Surf} + \text{T2R\_Surf} + \text{TGF\_beta}$	
22	R22_LRC_EE-_degradation		$\text{LRC\_EE} \longrightarrow \emptyset$	
23	R23_Smads-_Complex-_formation		$\text{Smad2c} + \text{Smad4c} \xrightarrow{\text{LRC\_EE}} \text{Smads\_Complex\_c}$	
24	R24_Smads-_Complex_import		$\text{Smads\_Complex\_c} \longrightarrow \text{Smads\_Complex\_n}$	
25	R25_Smads-_Complex-_Dissociation		$\text{Smads\_Complex\_n} \longrightarrow \text{Smad4n} + \text{Smad2n}$	
26	R26_LRC_Cave-_degradation		$\text{LRC\_Cave} \xrightarrow{\text{Smads\_Complex\_n}} \emptyset$	

7.1 Reaction R1_Smad2_import

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

Reaction equation

$$\text{Smad2c} \longrightarrow \text{Smad2n} \tag{3}$$

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

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

7.2 Reaction R2_Smad2_export

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

Reaction equation

$$\text{Smad2n} \longrightarrow \text{Smad2c} \tag{5}$$

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

$$v_2 = \mathrm{vol}\,(\mathrm{V\_nuc}) \cdot \mathrm{Kexp\_Smad2n} \cdot [\mathrm{Smad2n}] \tag{6}$$

7.3 Reaction R3_Smad4_import

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

Reaction equation

$$\mathrm{Smad4c} \longrightarrow \mathrm{Smad4n} \tag{7}$$

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

$$v_3 = \mathrm{vol}\,(\mathrm{V\_cyt}) \cdot \mathrm{Kimp\_Smad4c} \cdot [\mathrm{Smad4c}] \tag{8}$$

7.4 Reaction R4_Smad4_export

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

Reaction equation

$$\text{Smad4n} \longrightarrow \text{Smad4c} \tag{9}$$

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

$$v_4 = \text{vol}\,(\text{V\_nuc}) \cdot \text{Kexp\_Smad4n} \cdot [\text{Smad4n}] \tag{10}$$

7.5 Reaction R5_T1R_production

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

Reaction equation

$$\emptyset \longrightarrow \text{T1R\_Surf} \tag{11}$$

Product

Table 14: Properties of each product.

Id	Name	SBO
T1R_Surf	T1R_Surf	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\left(\mathrm{V\_cyt}\right) \cdot \mathrm{v\_T1R} \tag{12}$$

7.6 Reaction R6_T1R_Cave_formation

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

Reaction equation

$$\mathrm{T1R\_Surf} \longrightarrow \mathrm{T1R\_Cave} \tag{13}$$

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

$$v_6 = \mathrm{vol}\left(\mathrm{V\_cyt}\right) \cdot \mathrm{ki\_Cave} \cdot [\mathrm{T1R\_Surf}] \tag{14}$$

7.7 Reaction R7_T1R_Cave_recycling

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

Reaction equation

$$\mathrm{T1R\_Cave} \longrightarrow \mathrm{T1R\_Surf} \tag{15}$$

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

$$v_7 = \mathrm{vol}\,(\mathrm{V\_cyt}) \cdot \mathrm{kr\_Cave} \cdot [\mathrm{T1R\_Cave}] \tag{16}$$

7.8 Reaction R8_T1R_EE_formation

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

Reaction equation

$$\mathrm{T1R\_Surf} \longrightarrow \mathrm{T1R\_EE} \tag{17}$$

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

$$v_8 = \mathrm{vol}\,(\mathrm{V\_cyt}) \cdot \mathrm{ki\_EE} \cdot [\mathrm{T1R\_Surf}] \tag{18}$$

7.9 Reaction R9_T1R_EE_recycling

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

Reaction equation

$$\mathrm{T1R\_EE} \longrightarrow \mathrm{T1R\_Surf} \tag{19}$$

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

$$v_9 = \mathrm{vol}\,(\mathrm{V\_cyt}) \cdot \mathrm{kr\_EE} \cdot [\mathrm{T1R\_EE}] \tag{20}$$

7.10 Reaction R10_T1R_EE_degradation

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

Reaction equation

$$\mathrm{T1R\_EE} \longrightarrow \emptyset \tag{21}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
T1R_EE	T1R_EE	

Kinetic Law

Derived unit contains undeclared units

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

7.11 Reaction R11_T2R_production

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

Reaction equation

$$\emptyset \longrightarrow \mathrm{T2R\_Surf} \tag{23}$$

Product

Table 24: Properties of each product.

Id	Name	SBO
T2R_Surf	T2R_Surf	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}(\mathrm{V\_cyt}) \cdot \mathrm{v\_T2R} \tag{24}$$

7.12 Reaction R12_T2R_Cave_formation

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

Reaction equation

$$\mathrm{T2R\_Surf} \longrightarrow \mathrm{T2R\_Cave} \tag{25}$$

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

$$v_{12} = \mathrm{vol}\,(\mathrm{V\_cyt}) \cdot \mathrm{ki\_Cave} \cdot [\mathrm{T2R\_Surf}] \tag{26}$$

7.13 Reaction R13_T2R_Cave_recycling

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

Reaction equation

$$\mathrm{T2R\_Cave} \longrightarrow \mathrm{T2R\_Surf} \tag{27}$$

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

$$v_{13} = \mathrm{vol}\,(\mathrm{V\_cyt}) \cdot \mathrm{kr\_Cave} \cdot [\mathrm{T2R\_Cave}] \tag{28}$$

7.14 Reaction R14_T2R_EE_formation

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

Reaction equation

$$\mathrm{T2R\_Surf} \longrightarrow \mathrm{T2R\_EE} \tag{29}$$

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

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

7.15 Reaction R15_T2R_EE_recycling

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

Reaction equation

$$\mathrm{T2R\_EE} \longrightarrow \mathrm{T2R\_Surf} + \mathrm{TGF\_beta} \tag{31}$$

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

$$v_{15} = \mathrm{vol}\,(\mathrm{V\_cyt}) \cdot \mathrm{kr\_EE} \cdot [\mathrm{T2R\_EE}] \tag{32}$$

7.16 Reaction R16_T2R_EE_degradation

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

Reaction equation

$$\mathrm{T2R\_EE} \longrightarrow \emptyset \tag{33}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
T2R_EE	T2R_EE	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{V\_cyt}) \cdot \mathrm{Kdeg\_T2R\_EE} \cdot [\mathrm{T2R\_EE}] \tag{34}$$

7.17 Reaction R17_LRC_formation

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

Reaction equation

$$\text{TGF\_beta} + \text{T2R\_Surf} + \text{T1R\_Surf} \longrightarrow \text{LRC\_Surf} \tag{35}$$

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

$$v_{17} = \text{vol}(\text{V\_cyt}) \cdot \text{k\_LRC} \cdot [\text{TGF\_beta}] \cdot [\text{T2R\_Surf}] \cdot [\text{T1R\_Surf}] \tag{36}$$

7.18 Reaction R18_LRC_Cave_formation

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

Reaction equation

$$\text{LRC\_Surf} \longrightarrow \text{LRC\_Cave} \tag{37}$$

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

$$v_{18} = \mathrm{vol}(\mathrm{V\_cyt}) \cdot \mathrm{ki\_Cave} \cdot [\mathrm{LRC\_Surf}] \tag{38}$$

7.19 Reaction R19_LRC_Cave_recycling

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

Reaction equation

$$\mathrm{LRC\_Cave} \longrightarrow \mathrm{T1R\_Surf} + \mathrm{TGF\_beta} + \mathrm{T2R\_Surf} \tag{39}$$

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

$$v_{19} = \mathrm{vol}(\mathrm{V\_cyt}) \cdot \mathrm{kr\_Cave} \cdot [\mathrm{LRC\_Cave}] \tag{40}$$

7.20 Reaction R20_LRC_EE_formation

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

Reaction equation

$$\text{LRC\_Surf} \longrightarrow \text{LRC\_EE} \tag{41}$$

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

$$v_{20} = \text{vol}\left(\text{V\_cyt}\right) \cdot \text{ki\_EE} \cdot \left[\text{LRC\_Surf}\right] \tag{42}$$

7.21 Reaction R21_LRC_EE_recycling

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

Reaction equation

$$\text{LRC\_EE} \longrightarrow \text{T1R\_Surf} + \text{T2R\_Surf} + \text{TGF\_beta} \tag{43}$$

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

$$v_{21} = \mathrm{vol}\,(\mathrm{V\_cyt}) \cdot \mathrm{kr\_EE} \cdot [\mathrm{LRC\_EE}] \tag{44}$$

7.22 Reaction R22_LRC_EE_degradation

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

Reaction equation

$$\mathrm{LRC\_EE} \longrightarrow \emptyset \tag{45}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
LRC_EE	LRC_EE	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{vol}\,(\mathrm{V\_cyt}) \cdot \mathrm{Kcd} \cdot [\mathrm{LRC\_EE}] \tag{46}$$

7.23 Reaction R23_Smads_Complex_formation

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

Reaction equation

$$\mathrm{Smad2c} + \mathrm{Smad4c} \xrightarrow{\mathrm{LRC\_EE}} \mathrm{Smads\_Complex\_c} \tag{47}$$

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

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

7.24 Reaction R24_Smads_Complex_import

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

Reaction equation

$$\mathrm{Smads\_Complex\_c} \longrightarrow \mathrm{Smads\_Complex\_n} \tag{49}$$

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

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

7.25 Reaction R25_Smads_Complex_Dissociation

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

Reaction equation

$$\mathrm{Smads\_Complex\_n} \longrightarrow \mathrm{Smad4n} + \mathrm{Smad2n} \tag{51}$$

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

$$v_{25} = \mathrm{vol}\,(\mathrm{V\_nuc}) \cdot \mathrm{Kdiss\_Smads\_Complex\_n} \cdot [\mathrm{Smads\_Complex\_n}] \tag{52}$$

7.26 Reaction R26_LRC_Cave_degradation

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

Reaction equation

$$\mathrm{LRC\_Cave} \xrightarrow{\mathrm{Smads\_Complex\_n}} \emptyset \tag{53}$$

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

$$v_{26} = \mathrm{vol}\,(\mathrm{V\_cyt}) \cdot \mathrm{Klid} \cdot [\mathrm{LRC\_Cave}] \cdot [\mathrm{Smads\_Complex\_n}] \tag{54}$$

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 $492.61\ \mathrm{nmol \cdot l^{-1}}$

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`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Smad2c} = v_2 - v_1 - v_{23} \tag{55}$$

8.2 Species `Smad2n`

Name Smad2n

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

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`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Smad2n} = v_1 + v_{25} - v_2 \tag{56}$$

8.3 Species `Smad4c`

Name Smad4c

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

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`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Smad4c} = v_4 - v_3 - v_{23} \tag{57}$$

8.4 Species Smad4n

Name Smad4n

Initial concentration $551.72\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Smad4n} = v_3 + v_{25} - v_4 \tag{58}$$

8.5 Species T1R_Surf

Name T1R_Surf

Initial concentration $0.237\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T1R\_Surf} = v_5 + v_7 + v_9 + v_{19} + v_{21} - v_6 - v_8 - v_{17} \tag{59}$$

8.6 Species T1R_Cave

Name T1R_Cave

Initial concentration $2.092\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T1R\_Cave} = v_6 - v_7 \tag{60}$$

8.7 Species T1R_EE

Name T1R_EE

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T1R\_EE} = v_8 - v_9 - v_{10} \tag{61}$$

8.8 Species T2R_Surf

Name T2R_Surf

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T2R\_Surf} = v_{11} + v_{13} + v_{15} + v_{19} + v_{21} - v_{12} - v_{14} - v_{17} \tag{62}$$

8.9 Species T2R_Cave

Name T2R_Cave

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T2R\_Cave} = v_{12} - v_{13} \tag{63}$$

8.10 Species T2R_EE

Name T2R_EE

Initial concentration $1.148\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T2R\_EE} = v_{14} - v_{15} - v_{16} \tag{64}$$

8.11 Species LRC_Surf

Name LRC_Surf

Initial concentration $0\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{LRC\_Surf} = v_{17} - v_{18} - v_{20} \tag{65}$$

8.12 Species LRC_Cave

Name LRC_Cave

Initial concentration $0\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{LRC\_Cave} = v_{18} - v_{19} - v_{26} \tag{66}$$

8.13 Species LRC_EE

Name LRC_EE

Initial concentration $0\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{LRC\_EE} = v_{20} - v_{21} - v_{22} \tag{67}$$

8.14 Species Smads_Complex_c

Name Smads_Complex_c

Initial concentration $0\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Smads\_Complex\_c} = v_{23} - v_{24} \tag{68}$$

8.15 Species Smads_Complex_n

Name Smads_Complex_n

Initial concentration $0\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Smads\_Complex\_n} = v_{24} - v_{25} \tag{69}$$

8.16 Species TGF_beta

Name TGF_beta

Initial concentration $0.08\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TGF\_beta} = v_{15} + v_{19} + v_{21} - v_{17} \tag{70}$$

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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