SBML Model Report

Model name: "Kallenberger2014 - CD95L induced apoptosis initiated by caspase-8, wild-type HeLa cells (cis/trans-cis/trans variant)"



May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah¹ and Stefan Kallenberger² at March 14th 2014 at 12:53 a.m. and last time modified at February 25th 2015 at 12:39 a.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	18
events	0	constraints	0
reactions	19	function definitions	0
global parameters	15	unit definitions	0
rules	1	initial assignments	0

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Model Notes

Kallenberger2014 - CD95L induced apoptosis initiated by caspase-8, wild-type HeLa cells (cis/trans-cis/trans variant)

The paper describes a new approach that combines single cell and population data in the same model. The model consists of a large number of single cell models, which are fitted to single cell data. Simultaneously, ensemble averages are fitted to population data. It is assumed that the kinetics in each cell can be described with the same kinetic parameters. Therefore, cell-to-cell variability is explained by variable initial protein concentrations.

There are four variants of the model (with [CD95L]=500ng/ml = 16.6nM), i) cistrans (in CD95-HeLa cells) [MODEL1403050000], ii) cistrans (in wild-type HeLa cells) [MODEL1403050001], iii) cistrans-cistrans (in CD95-HeLa cells) [MODEL1403050002], and iv) cistrans-cistrans (in wild-type HeLa cells) [MODEL1403050003].

These model contain the equations for one "average cell,, with median initial concentrations for CD95, FADD, p55, BID, PrNES_mCherry and PrER_mGFP. By integrating the model, it should be possible to obtain trajectories for PrER_mGFP, PrNES_mCherry, p43 and p18 similar as in Figure 4A (CD95-HeLa cells) and Figure 4B (wild-type HeLa cells).

This model is described in the article:Intra- and Interdimeric Caspase-8 Self-Cleavage Controls Strength and Timing of CD95-Induced ApoptosisStefan M. Kallenberger, Jol Beaudouin, Juliane Claus, Carmen Fischer, Peter K. Sorger, Stefan Legewie, and Roland Eils11 March 2014: Vol. 7, Issue 316, p. ra23

Abstract:

Apoptosis in response to the ligand CD95L (also known as Fas ligand) is initiated by caspase-8, which is activated by dimerization and self-cleavage at death-inducing signaling complexes (DISCs). Previous work indicated that the degree of substrate cleavage by caspase-8 determines whether a cell dies or survives in response to a death stimulus. To determine how a death ligand stimulus is effectively translated into caspase-8 activity, we assessed this activity over time in single cells with compartmentalized probes that are cleaved by caspase-8 and used multiscale modeling to simultaneously describe single-cell and population data with an ensemble of singlecell models. We derived and experimentally validated a minimal model in which cleavage of caspase-8 in the enzymatic domain occurs in an interdimeric manner through interaction between DISCs, whereas prodomain cleavage sites are cleaved in an intradimeric manner within DISCs. Modeling indicated that sustained membrane-bound caspase-8 activity is followed by transient cytosolic activity, which can be interpreted as a molecular timer mechanism reflected by a limited lifetime of active caspase-8. The activation of caspase-8 by combined intra- and interdimeric cleavage ensures weak signaling at low concentrations of CD95L and strongly accelerated activation at higher ligand concentrations, thereby contributing to precise control of apoptosis.

This model is hosted on BioModels Database and identifiedby: BIOMD0000000526.

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

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2 Unit Definitions

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

2.1 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

2.2 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.3 Unit area

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

Definition m^2

2.4 Unit length

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

Definition m

2.5 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cell	cell		3	1	litre	Z	

3.1 Compartment cell

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

Name cell

4 Species

This model contains 18 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 Condi- tion
CD95	CD95	cell	$\text{mol} \cdot 1^{-1}$		
FADD	FADD	cell	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		\Box
p55free	p55free	cell	$\operatorname{mol} \cdot 1^{-1}$		\Box
Bid	Bid	cell	$\operatorname{mol} \cdot 1^{-1}$		\Box
PrNES_mCherry	PrNES_mCherry	cell	$\operatorname{mol} \cdot 1^{-1}$		
PrER_mGFP	PrER_mGFP	cell	$\operatorname{mol} \cdot 1^{-1}$		
DISC	DISC	cell	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		
DISCp55	DISCp55	cell	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		
p30	p30	cell	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		\Box
p43	p43	cell	$\operatorname{mol} \cdot 1^{-1}$		
p18	p18	cell	$\operatorname{mol} \cdot 1^{-1}$		
p18inactive	p18inactive	cell	$\operatorname{mol} \cdot 1^{-1}$		
tBid	tBid	cell	$\operatorname{mol} \cdot 1^{-1}$		
PrNES	PrNES	cell	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		
mCherry	mCherry	cell	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		
PrER	PrER	cell	$\operatorname{mol} \cdot 1^{-1}$		
mGFP	mGFP	cell	$\text{mol} \cdot l^{-1}$		
CD95L	CD95L	cell	$\operatorname{mol} \cdot 1^{-1}$		

5 Parameters

This model contains 15 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kon_FADD			0.001		$\overline{\hspace{1cm}}$
$koff_FADD$			0.001		$\overline{\mathbf{Z}}$
kDISC		3.6	4965874405544 - 1	10^{-4}	$ \overline{\mathbf{Z}} $
kD216			0.006		$ \overline{\mathbf{Z}} $
kD216trans- _p55		2.2	3246421372882 · 1	10^{-4}	
kD216trans- _p43		5.2	9906975294056 · 1	10^{-5}	\square
kD374		6.4	4612643975149 - 1	10^{-4}	
kD374trans- _p55		5.4	3518631342483 · 1	10^{-4}	\mathbf{Z}
kD374trans- _p43			0.004		\square
kdiss_p18			0.065		
kBid		5.	2134055139547 - 1	10^{-4}	$\overline{\mathbf{Z}}$
kD374probe			0.002		$\overline{\mathbf{Z}}$
KDR			57.205		$\overline{\mathbf{Z}}$
KDL			30.006		\overline{Z}
CD95act			0.000		

6 Rule

This is an overview of one rule.

6.1 Rule CD95act

Rule CD95act is an assignment rule for parameter CD95act:

$$\begin{aligned} & \text{CD95act} \\ &= \frac{[\text{CD95}]^3 \cdot \text{KDL}^2 \cdot [\text{CD95L}]}{([\text{CD95L}] + \text{KDL}) \cdot \left([\text{CD95}]^2 \cdot \text{KDL}^2 + \text{KDR} \cdot [\text{CD95L}]^2 + 2 \cdot \text{KDR} \cdot \text{KDL} \cdot [\text{CD95L}] + \text{KDR} \cdot \text{KDL}^2\right)} \end{aligned}$$

7 Reactions

This model contains 19 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

N₀	Id N	Jame	Reaction Equation	SBO
1	reaction_1		$FADD \xrightarrow{FADD} DISC$	
2	reaction_2	1	$\operatorname{DISC} \xrightarrow{\operatorname{DISC}} \operatorname{FADD}$	
3	reaction_3		$p55free + DISC \xrightarrow{p55free, DISC} DISCp55$	
4	reaction_4		DISCp55 $\xrightarrow{\text{DISCp55}}$ p30	
5	reaction_5	1	DISCp55 $\xrightarrow{\text{DISCp55}, p30, DISCp55, p30}$ p30	
6	reaction_6	1	DISCp55 $\xrightarrow{\text{p43, DISCp55, p43}}$ p30	
7	reaction_7		$p43 \xrightarrow{p43} p18 + DISC$	
8	reaction_8	1	p43 DISCp55, p30, p43, DISCp55, p30 + p18 +	-
			DISC	
9	reaction_9	1	$p43 \xrightarrow{p43, p43} p18 + DISC$	
10	reaction_10	J	DISCp55 $\xrightarrow{\text{DISCp55}}$ p43	
11	reaction_11]	DISCp55 $\xrightarrow{\text{DISCp55}, p30, DISCp55, p30}$ p43	
12	reaction_12	J	DISCp55 $\xrightarrow{\text{p43}}$ DISCp55, p43 $\xrightarrow{\text{p43}}$ p43	
13	reaction_13	J	$p30 \xrightarrow{p30} p18 + DISC$	
14	reaction_14		p30 DISCp55, p30, p30, DISCp55 p18 + DISC	
15	reaction_15	1	$p30 \xrightarrow{p43, p30, p43} p18 + DISC$	

N⁰	Id	Name	Reaction Equation	SBO
16	reaction_16		p18 $\xrightarrow{p18}$ p18inactive	
17	reaction_17		$Bid \xrightarrow{p43, p18, Bid, p43, p18} tBid$	
18	reaction_18		PrNES_mCherry p43, p18, PrNES_mCherry, p43, p1	$\stackrel{8}{\rightarrow}$ PrNES +
			mCherry	
19	reaction_19		$PrER_mGFP \xrightarrow{p18, PrER_mGFP, p18} PrER + mGFP$	

7.1 Reaction reaction_1

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

Reaction equation

$$FADD \xrightarrow{FADD} DISC \tag{2}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
FADD	FADD	

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
FADD	FADD	

Product

Table 8: Properties of each product.

Id	Name	SBO
DISC	DISC	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{kon_FADD} \cdot \text{CD95act} \cdot [\text{FADD}] \cdot \text{vol}(\text{cell})$$
 (3)

7.2 Reaction reaction_2

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

Reaction equation

$$DISC \xrightarrow{DISC} FADD \tag{4}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
DISC	DISC	

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
DISC	DISC	

Product

Table 11: Properties of each product.

Id	Name	SBO
FADD	FADD	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{koff_FADD} \cdot [\text{DISC}] \cdot \text{vol} (\text{cell})$$
 (5)

7.3 Reaction reaction_3

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

Reaction equation

$$p55free + DISC \xrightarrow{p55free, DISC} DISCp55$$
 (6)

Table 12: Properties of each reactant.

Id	Name	SBO
p55free	p55free	

Id	Name	SBO
DISC	DISC	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
p55free DISC	p55free DISC	

Product

Table 14: Properties of each product.

Id	Name	SBO
DISCp55	DISCp55	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{kDISC} \cdot [\text{p55free}] \cdot [\text{DISC}] \cdot \text{vol} (\text{cell})$$
 (7)

7.4 Reaction reaction_4

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

Reaction equation

$$DISCp55 \xrightarrow{DISCp55} p30 \tag{8}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
DISCp55	DISCp55	

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
DISCp55	DISCp55	

Product

Table 17: Properties of each product.

Id	Name	SBO
p30	p30	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{kD216} \cdot [\text{DISCp55}] \cdot \text{vol(cell)} \tag{9}$$

7.5 Reaction reaction_5

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

Reaction equation

$$DISCp55 \xrightarrow{DISCp55, p30, DISCp55, p30} p30$$
 (10)

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
DISCp55	DISCp55	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
DISCp55	DISCp55	
p30	p30	
DISCp55	DISCp55	

Id	Name	SBO
p30	p30	

Product

Table 20: Properties of each product.

Id	Name	SBO
p30	p30	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{kD216trans_p55} \cdot [\text{DISCp55}] \cdot ([\text{DISCp55}] + [\text{p30}]) \cdot \text{vol}(\text{cell})$$
 (11)

7.6 Reaction reaction_6

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

Reaction equation

$$DISCp55 \xrightarrow{p43, DISCp55, p43} p30$$
 (12)

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
DISCp55	DISCp55	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
p43 DISCp55 p43	p43 DISCp55 p43	

Product

Table 23: Properties of each product.

Id	Name	SBO
p30	p30	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{kD216trans_p43} \cdot [\text{DISCp55}] \cdot [\text{p43}] \cdot \text{vol} (\text{cell})$$
(13)

7.7 Reaction reaction_7

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

Reaction equation

$$p43 \xrightarrow{p43} p18 + DISC \tag{14}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
p43	p43	

Modifier

Table 25: Properties of each modifier.

Id	Name	SBO
p43	p43	

Products

Table 26: Properties of each product.

Id	Name	SBO
p18	p18	

Id	Name	SBO
DISC	DISC	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{kD216} \cdot [\text{p43}] \cdot \text{vol}(\text{cell}) \tag{15}$$

7.8 Reaction reaction_8

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

Reaction equation

$$p43 \xrightarrow{DISCp55, p30, p43, DISCp55, p30} p18 + DISC$$
 (16)

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
p43	p43	

Modifiers

Table 28: Properties of each modifier.

Id	Name	SBO
DISCp55	DISCp55	
p30	p30	
p43	p43	
DISCp55	DISCp55	
p30	p30	

Products

Table 29: Properties of each product.

Id	Name	SBO
p18	p18	

Id	Name	SBO
DISC	DISC	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{kD216trans_p55} \cdot [\text{p43}] \cdot ([\text{DISCp55}] + [\text{p30}]) \cdot \text{vol}(\text{cell})$$
(17)

7.9 Reaction reaction_9

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

Reaction equation

$$p43 \xrightarrow{p43, p43} p18 + DISC$$
 (18)

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
p43	p43	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
p43	p43	
p43	p43	

Products

Table 32: Properties of each product.

Id	Name	SBO
p18 DISC	p18 DISC	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{kD216trans_p43} \cdot [\text{p43}] \cdot [\text{p43}] \cdot \text{vol(cell)}$$
(19)

7.10 Reaction reaction_10

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

Reaction equation

$$DISCp55 \xrightarrow{DISCp55} p43 \tag{20}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
DISCp55	DISCp55	

Modifier

Table 34: Properties of each modifier.

Id	Name	SBO
DISCp55	DISCp55	

Product

Table 35: Properties of each product.

Id	Name	SBO
p43	p43	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{kD374} \cdot [\text{DISCp55}] \cdot \text{vol} (\text{cell})$$
 (21)

7.11 Reaction reaction_11

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

Reaction equation

$$DISCp55 \xrightarrow{DISCp55, p30, DISCp55, p30} p43$$
 (22)

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
DISCp55	DISCp55	

Modifiers

Table 37: Properties of each modifier.

Id	Name	SBO
DISCp55	DISCp55	
p30	p30	
DISCp55	DISCp55	
p30	p30	

Product

Table 38: Properties of each product.

Id	Name	SBO
p43	p43	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{kD374trans_p55} \cdot [\text{DISCp55}] \cdot ([\text{DISCp55}] + [\text{p30}]) \cdot \text{vol}(\text{cell})$$
 (23)

7.12 Reaction reaction_12

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

Reaction equation

$$DISCp55 \xrightarrow{p43, DISCp55, p43} p43$$
 (24)

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
DISCp55	DISCp55	

Modifiers

Table 40: Properties of each modifier.

Id	Name	SBO
p43 DISCp55 p43	p43 DISCp55 p43	

Product

Table 41: Properties of each product.

Id	Name	SBO
p43	p43	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{kD374trans_p43} \cdot [\text{DISCp55}] \cdot [\text{p43}] \cdot \text{vol} (\text{cell})$$
 (25)

7.13 Reaction reaction_13

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

Reaction equation

$$p30 \xrightarrow{p30} p18 + DISC \tag{26}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
p30	p30	

Modifier

Table 43: Properties of each modifier.

Id	Name	SBO
p30	p30	

Products

Table 44: Properties of each product.

Id	Name	SBO
p18 DISC	p18 DISC	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{kD374} \cdot [\text{p30}] \cdot \text{vol} (\text{cell})$$
 (27)

7.14 Reaction reaction_14

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

Reaction equation

$$p30 \xrightarrow{DISCp55, p30, p30, DISCp55} p18 + DISC \tag{28}$$

Table 45: Properties of each reactant.

Id	Name	SBO
p30	p30	

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
DISCp55	DISCp55	
p30	p30	
p30	p30	
DISCp55	DISCp55	

Products

Table 47: Properties of each product.

Id	Name	SBO
p18 DISC	p18 DISC	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{kD374trans_p55} \cdot [\text{p30}] \cdot ([\text{DISCp55}] + [\text{p30}]) \cdot \text{vol} (\text{cell})$$
 (29)

7.15 Reaction reaction_15

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

Reaction equation

$$p30 \xrightarrow{p43, p30, p43} p18 + DISC$$
 (30)

Table 48: Properties of each reactant.

Id	Name	SBO
p30	p30	

Modifiers

Table 49: Properties of each modifier.

Id	Name	SBO
p43	p43 p30	
p30 p43	p30 p43	
	•	

Products

Table 50: Properties of each product.

Id	Name	SBO
p18 DISC	p18 DISC	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{kD374trans_p43} \cdot [\text{p30}] \cdot [\text{p43}] \cdot \text{vol} (\text{cell})$$
(31)

7.16 Reaction reaction_16

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

Reaction equation

$$p18 \xrightarrow{p18} p18 inactive \tag{32}$$

Table 51: Properties of each reactant.

Id	Name	SBO
p18	p18	

Modifier

Table 52: Properties of each modifier.

Id	Name	SBO
p18	p18	

Product

Table 53: Properties of each product.

Id	Name	SBO
p18inactive	p18inactive	-

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{kdiss_p18} \cdot [\text{p18}] \cdot \text{vol} (\text{cell})$$
(33)

7.17 Reaction reaction_17

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

Reaction equation

$$Bid \xrightarrow{p43, p18, Bid, p43, p18} tBid$$
 (34)

Table 54: Properties of each reactant.

Id	Name	SBO
Bid	Bid	

Modifiers

Table 55: Properties of each modifier.

Id	Name	SBO
p43	p43	
p18	p18	
Bid	Bid	
p43	p43	
p18	p18	

Product

Table 56: Properties of each product.

Id	Name	SBO
tBid	tBid	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{kBid} \cdot [\text{Bid}] \cdot ([\text{p43}] + [\text{p18}]) \cdot \text{vol}(\text{cell})$$
(35)

7.18 Reaction reaction_18

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

Reaction equation

$$PrNES_mCherry \xrightarrow{p43, p18, PrNES_mCherry, p43, p18} PrNES + mCherry$$
 (36)

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
PrNES_mCherry	PrNES_mCherry	

Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
p43	p43	
p18	p18	
PrNES_mCherry	PrNES_mCherry	
p43	p43	
p18	p18	

Products

Table 59: Properties of each product.

Id	Name	SBO
PrNES	PrNES	
${\tt mCherry}$	mCherry	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{kD374probe} \cdot [\text{PrNES_mCherry}] \cdot ([\text{p43}] + [\text{p18}]) \cdot \text{vol}(\text{cell})$$
 (37)

7.19 Reaction reaction_19

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

Reaction equation

$$PrER_mGFP \xrightarrow{p18, PrER_mGFP, p18} PrER + mGFP$$
 (38)

Reactant

Table 60: Properties of each reactant.

Id	Name	SBO
PrER_mGFP	PrER_mGFP	

Modifiers

Table 61: Properties of each modifier.

Id	Name	SBO
p18 PrER_mGFP p18	p18 PrER_mGFP p18	

Products

Table 62: Properties of each product.

Id	Name	SBO
PrER	PrER	
mGFP	mGFP	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{kD374probe} \cdot [\text{PrER_mGFP}] \cdot [\text{p18}] \cdot \text{vol}(\text{cell})$$
 (39)

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 CD95

Name CD95

Initial concentration $12 \text{ mol} \cdot l^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CD95} = 0\tag{40}$$

8.2 Species FADD

Name FADD

Initial concentration $90 \text{ mol} \cdot l^{-1}$

This species takes part in three reactions (as a reactant in reaction_1 and as a product in reaction_2 and as a modifier in reaction_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FADD} = v_2 - v_1 \tag{41}$$

8.3 Species p55free

Name p55free

Initial concentration $127 \text{ mol} \cdot l^{-1}$

This species takes part in two reactions (as a reactant in reaction_3 and as a modifier in reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{p55free} = -\nu_3\tag{42}$$

8.4 Species Bid

Name Bid

Initial concentration 224 mol·1⁻¹

This species takes part in two reactions (as a reactant in reaction_17 and as a modifier in reaction_17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bid} = -v_{17} \tag{43}$$

8.5 Species PrNES_mCherry

Name PrNES_mCherry

Initial concentration $1909 \text{ mol} \cdot l^{-1}$

This species takes part in two reactions (as a reactant in reaction_18 and as a modifier in reaction_18).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{PrNES_mCherry} = -v_{18} \tag{44}$$

8.6 Species PrER_mGFP

Name PrER_mGFP

Initial concentration 3316 mol·l⁻¹

This species takes part in two reactions (as a reactant in reaction_19 and as a modifier in reaction_19).

$$\frac{d}{dt} PrER_mGFP = -v_{19}$$
 (45)

8.7 Species DISC

Name DISC

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

This species takes part in eleven reactions (as a reactant in reaction_2, reaction_3 and as a product in reaction_1, reaction_7, reaction_8, reaction_9, reaction_13, reaction_14, reaction_15 and as a modifier in reaction_2, reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{DISC} = |v_1| + |v_7| + |v_8| + |v_9| + |v_{13}| + |v_{14}| + |v_{15}| - |v_2| - |v_3| \tag{46}$$

8.8 Species DISCp55

Name DISCp55

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

This species takes part in 19 reactions (as a reactant in reaction_4, reaction_5, reaction_6, reaction_10, reaction_11, reaction_12 and as a product in reaction_3 and as a modifier in reaction_4, reaction_5, reaction_5, reaction_6, reaction_8, reaction_8, reaction_11, reaction_11, reaction_12, reaction_14, reaction_14).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{DISCp55} = |v_3| - |v_4| - |v_5| - |v_6| - |v_{10}| - |v_{11}| - |v_{12}| \tag{47}$$

8.9 Species p30

Name p30

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

This species takes part in 16 reactions (as a reactant in reaction_13, reaction_14, reaction_15 and as a product in reaction_4, reaction_5, reaction_6 and as a modifier in reaction_5, reaction_5, reaction_8, reaction_11, reaction_11, reaction_13, reaction_14, reaction_14, reaction_15).

$$\frac{\mathrm{d}}{\mathrm{d}t}p30 = |v_4| + |v_5| + |v_6| - |v_{13}| - |v_{14}| - |v_{15}| \tag{48}$$

8.10 Species p43

Name p43

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

This species takes part in 20 reactions (as a reactant in reaction_7, reaction_8, reaction_9 and as a product in reaction_10, reaction_11, reaction_12 and as a modifier in reaction_6, reaction_6, reaction_7, reaction_8, reaction_9, reaction_9, reaction_12, reaction_12, reaction_12, reaction_13, reaction_14, reaction_15, reaction_15, reaction_16, reaction_17, reaction_17, reaction_18, reaction_18).

$$\frac{\mathrm{d}}{\mathrm{d}t}p43 = |v_{10}| + |v_{11}| + |v_{12}| - |v_{7}| - |v_{8}| - |v_{9}| \tag{49}$$

8.11 Species p18

Name p18

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

This species takes part in 14 reactions (as a reactant in reaction_16 and as a product in reaction_7, reaction_8, reaction_9, reaction_13, reaction_14, reaction_15 and as a modifier in reaction_16, reaction_17, reaction_17, reaction_18, reaction_19, reaction_19).

$$\frac{d}{dt}p18 = |v_7| + |v_8| + |v_9| + |v_{13}| + |v_{14}| + |v_{15}| - |v_{16}|$$
(50)

8.12 Species p18inactive

Name p18inactive

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

This species takes part in one reaction (as a product in reaction_16).

$$\frac{\mathrm{d}}{\mathrm{d}t} p18 \text{inactive} = v_{16} \tag{51}$$

8.13 Species tBid

Name tBid

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

This species takes part in one reaction (as a product in reaction_17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{tBid} = v_{17} \tag{52}$$

8.14 Species PrNES

Name PrNES

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

This species takes part in one reaction (as a product in reaction_18).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{PrNES} = v_{18} \tag{53}$$

8.15 Species mCherry

Name mCherry

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

This species takes part in one reaction (as a product in reaction_18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{mCherry} = v_{18} \tag{54}$$

8.16 Species PrER

Name PrER

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

This species takes part in one reaction (as a product in reaction_19).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{PrER} = v_{19} \tag{55}$$

8.17 Species mGFP

Name mGFP

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

This species takes part in one reaction (as a product in reaction_19).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{mGFP} = v_{19} \tag{56}$$

8.18 Species CD95L

Name CD95L

Initial concentration $16.6 \text{ mol} \cdot l^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CD95L} = 0\tag{57}$$

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