SBML Model Report

Model name: "Albeck2008_extrinsic_apoptosis"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Lukas Endler[1] and Simon Fourquet[2] at July first 2009 at 5:12 p. m. and last time modified at February 25th 2015 at 12:42 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	2
species types	0	species	58
events	0	constraints	0
reactions	42	function definitions	0
global parameters	77	unit definitions	0
rules	6	initial assignments	0

Model Notes

This the model used in the article:
Quantitative analysis of pathways controlling extrinsic apoptosis in single cells.
Albeck JG, Burke JM, Aldridge BB, Zhang M, Lauffenburger DA, Sorger PK. Mol Cell. 2008 Apr 11;30(1):11-25. PMID: 18406323 , doi: 10.1016/j.molcel.2008.02.012

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Abstract:
Apoptosis in response to TRAIL or TNF requires the activation of initiatorcaspases, which then activate the effector caspases that dismantlecells and cause death. However, little is known about the dynamicsand regulatory logic linking initiators and effectors. Using a combinationof live-cell reporters, flow cytometry, and immunoblotting, we findthat initiator caspases are active during the long and variable delaythat precedes mitochondrial outer membrane permeabilization (MOMP)and effector caspase activation. When combined with a mathematicalmodel of core apoptosis pathways, experimental perturbation of regulatorylinks between initiator and effector caspases reveals that XIAP andproteasome-dependent degradation of effector caspases are importantin restraining activity during the pre-MOMP delay. We identify conditionsin which restraint is impaired, creating a physiologically indeterminatestate of partial cell death with the potential to generate genomicinstability. Together, these findings provide a quantitative pictureof caspase regulatory networks and their failure modes.
The mitochondrial compartment is just added as a logical partition and its volume is not used in the mathematical formulas, to stick closer to the expressions used in the matlab files distributed with the original publication. There only the rate constants for bimolecular reactions are adapted by division by $\underline{v}$, the ration of the volumes of the mitochondrial compartment and the total cell. For BCL2 overexpression in figure 5, the initial BCL2 amount was increased by a factor 12 to $2.4*10^{5}$. For siRNA downregulation of XIAP its amount was multiplied by 0.13 to $1.3*10^{4}$.

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 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 l

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 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

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

3.1 Compartment cell

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

Name cell

3.2 Compartment mitochondrion

This is a three dimensional compartment with a constant size of one litre, which is surrounded by cell (cell).

Name mitochondrion

4 Species

This model contains 58 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
L	L	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
R	R	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
flip	flip	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
pC8	proC8	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C8	casp8	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C6	casp6	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
BAR	BAR	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
pC3	proC3	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C3	casp3	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bid	Bid	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
tBid	tBid	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
pC6	proC6	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
XIAP	XIAP	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C3_Ub	Ub C3	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PARP	PARP	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CPARP	cPARP	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Smac	Smac	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bcl2c	cytosolic Bcl-2	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bax	Bax	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bax_hash	Bax#	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bcl2	Bcl-2	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
L_R	L:R	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
R_hash	R#	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
flip_R_hash	flip:R#	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
R_hash_pC8	R#:pC8	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C6_pC8	C6:pC8	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
BAR_C8	BAR:C8	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C8_pC3	C8:pC3	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
pC3_Apop	pC3:Apop	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Apop	Apop	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C8_Bid	C8:Bid	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C3_pC6	C3:pC6	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
XIAP_C3	XIAP:C3	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PARP_C3	PARP:C3	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Apop_XIAP	Apop:XIAP	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Smac_XIAP	Smac:XIAP	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bcl2c_tBid	Bcl2c:tBid	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bax_tBid	Bax:tBid	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Baxm_Bcl2	Baxm:Bcl2	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bax4	Bax4	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bax2_Bcl2	Bax2:Bcl2	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bax4_Bcl2	Bax4:Bcl2	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
M	M	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bax4_M	Bax4:M	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
M_hash	M#	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Smacm	Smac_m	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
M_hash_Smacm	M#:Smac_m	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Smacr	Smac released	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CytoCm	CytoC_m	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
M_hash_CytoCm	M#:CytoC_m	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CytoCr	CytoC released	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CytoC	CytoC	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Apaf	Apaf	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CytoC_Apaf	CytoC:Apaf	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Apaf_hash	Apaf#	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
pC9	proC9	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Baxm	Baxm	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bax2	Bax2	mitochondrion	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 77 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$4 \cdot 10^{-7}$		☑
k_1	k_1		0.001		☑
kc1	kc1		10^{-5}		☑
k2	k2		10^{-6}		☑
k_2	k_2		0.001		☑
k3	k3		10^{-6}		☑
k_3	k_3		0.001		☑
kc3	kc3		1.000		☑
k4	k4		10^{-6}		☑
k_4	k_4		0.001		☑
k5	k5		10^{-7}		☑
k_5	k_5		0.001		☑
kc5	kc5		1.000		☑
k6	k6		10^{-6}		☑
k_6	k_6		0.001		☑
kc6	kc6		1.000		☑
k7	k7		$3 \cdot 10^{-8}$		☑
k_7	k_7		0.001		☑
k8	k8		$2 \cdot 10^{-6}$		☑
k_8	k_8		0.001		☑
kc8	kc8		0.100		☑
k9	k9		10^{-6}		☑
k_9	k_9		0.010		☑
kc9	kc9		1.000		☑
k10	k10		10^{-7}		☑
k_10	k_10		0.001		☑
kc10	kc10		1.000		☑
k11	k11		10^{-6}		☑
k_11	k_11		0.001		☑
k12	k12		10^{-7}		☑
k_12	k_12		0.001		☑
kc12	kc12		1.000		☑
k13	k13		0.010		☑
k_13	k_13		0.010		☑
k14	k14		10^{-6}		☑
k_14	k_14		0.001		☑
k15	k15		10^{-6}		☑

Id	Name	SBO	Value	Unit	Constant
k_15	k_15		0.001		☑
k16	k16		10^{-6}		☑
k_16	k_16		0.001		☑
k17	k17		10^{-6}		☑
k_17	k_17		0.001		☑
k18	k18		10^{-6}		☑
k_18	k_18		0.001		☑
k19	k19		10^{-6}		☑
k_19	k_19		0.001		☑
kc19	kc19		1.000		☑
k20	k20		$2 \cdot 10^{-6}$		☑
k_20	k_20		0.001		☑
kc20	kc20		10.000		☑
k21	k21		$2 \cdot 10^{-6}$		☑
k_21	k_21		0.001		☑
kc21	kc21		10.000		☑
k22	k22		0.010		☑
k_22	k_22		0.010		☑
k23	k23		$5 \cdot 10^{-7}$		☑
k_23	k_23		0.001		☑
kc23	kc23		1.000		☑
k24	k24		$5 \cdot 10^{-8}$		☑
k_24	k_24		0.001		☑
k25	k25		$5 \cdot 10^{-9}$		☑
k_25	k_25		0.001		☑
kc25	kc25		1.000		☑
k26	k26		0.010		☑
k_26	k_26		0.010		☑
k27	k27		$2 \cdot 10^{-6}$		☑
k_27	k_27		0.001		☑
k28	k28		$7 \cdot 10^{-6}$		☑
k_28	k_28		0.001		☑
kc7	kc7		1.000		☑
v	v		0.070		☑
pC3_frac	pC3 fraction		0.000		⊟
C3_frac	C3 fraction		0.000		⊟
C3_UB_frac	degraded C3 fraction		0.000		⊟
cPARP_frac	cPARP fraction		0.000		⊟
C3_tot	total Caspase 3		0.000		⊟
fC3_fract	free C3 fraction		0.000		⊟

6 Rules

This is an overview of six rules.

6.1 Rule C3_tot

Rule C3_tot is an assignment rule for parameter C3_tot:

$$\begin{aligned} \text{C3\_tot} = {} & [\text{pC3}] + [\text{C8\_pC3}] + [\text{pC3\_Apop}] + [\text{C3}] \\ & + [\text{C3\_pC6}] + [\text{XIAP\_C3}] + [\text{PARP\_C3}] + [\text{C3\_Ub}] \end{aligned} \tag{1}$$

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

6.2 Rule C3_frac

Rule C3_frac is an assignment rule for parameter C3_frac:

$$\text{C3\_frac} = \frac{[\text{C3}] + [\text{C3\_pC6}] + [\text{XIAP\_C3}] + [\text{PARP\_C3}]}{\text{C3\_tot}} \tag{2}$$

6.3 Rule C3_UB_frac

Rule C3_UB_frac is an assignment rule for parameter C3_UB_frac:

$$\text{C3\_UB\_frac} = \frac{[\text{C3\_Ub}]}{\text{C3\_tot}} \tag{3}$$

6.4 Rule pC3_frac

Rule pC3_frac is an assignment rule for parameter pC3_frac:

$$\text{pC3\_frac} = \frac{[\text{pC3}] + [\text{C8\_pC3}] + [\text{pC3\_Apop}]}{\text{C3\_tot}} \tag{4}$$

6.5 Rule fC3_fract

Rule fC3_fract is an assignment rule for parameter fC3_fract:

$$\text{fC3\_fract} = \frac{[\text{C3}]}{\text{C3\_tot}} \tag{5}$$

6.6 Rule cPARP_frac

Rule cPARP_frac is an assignment rule for parameter cPARP_frac:

$$\text{cPARP\_frac} = \frac{[\text{CPARP}]}{[\text{CPARP}] + [\text{PARP}] + [\text{PARP\_C3}]} \tag{6}$$

Derived unit dimensionless

7 Reactions

This model contains 42 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	re1		$L + R \rightleftharpoons L\_R$	
2	re2		$L\_R \longrightarrow R\_hash$	
3	re3		$R\_hash + flip \rightleftharpoons flip\_R\_hash$	
4	re4		$R\_hash + pC8 \rightleftharpoons R\_hash\_pC8$	
5	re5		$R\_hash\_pC8 \longrightarrow C8 + R\_hash$	
6	re6		$C6 + pC8 \rightleftharpoons C6\_pC8$	
7	re7		$C6\_pC8 \longrightarrow C8 + C6$	
8	re8		$C8 + BAR \rightleftharpoons BAR\_C8$	
9	re9		$pC3 + C8 \rightleftharpoons C8\_pC3$	
10	re10		$C8\_pC3 \longrightarrow C8 + C3$	
11	re11		$C8 + Bid \rightleftharpoons C8\_Bid$	
12	re12		$C8\_Bid \longrightarrow tBid + C8$	
13	re13		$pC3 + Apop \rightleftharpoons pC3\_Apop$	
14	re14		$pC3\_Apop \longrightarrow C3 + Apop$	
15	re15		$C3 + pC6 \rightleftharpoons C3\_pC6$	
16	re16		$C3\_pC6 \longrightarrow C3 + C6$	
17	re17		$C3 + XIAP \rightleftharpoons XIAP\_C3$	
18	re18		$XIAP\_C3 \longrightarrow C3\_Ub + XIAP$	
19	re19		$PARP + C3 \rightleftharpoons PARP\_C3$	
20	re20		$PARP\_C3 \longrightarrow CPARP + C3$	
21	re21		$XIAP + Apop \rightleftharpoons Apop\_XIAP$	
22	re22		$XIAP + Smac \rightleftharpoons Smac\_XIAP$	
23	re23		$tBid + Bcl2c \rightleftharpoons Bcl2c\_tBid$	

№	Id	Name	Reaction Equation	SBO
24	re24		$\mathrm{tBid} + \mathrm{Bax} \rightleftharpoons \mathrm{Bax\_tBid}$	
25	re25		$\mathrm{Bax\_tBid} \longrightarrow \mathrm{tBid} + \mathrm{Bax\_hash}$	
26	re26		$\mathrm{Bax\_hash} \rightleftharpoons \mathrm{Baxm}$	
27	re27		$\mathrm{Baxm} + \mathrm{Bcl2} \rightleftharpoons \mathrm{Baxm\_Bcl2}$	
28	re29		$\mathrm{Baxm} + \mathrm{Baxm} \rightleftharpoons \mathrm{Bax2}$	
29	re30		$\mathrm{Bax2} + \mathrm{Bax2} \rightleftharpoons \mathrm{Bax4}$	
30	re31		$\mathrm{Bcl2} + \mathrm{Bax2} \rightleftharpoons \mathrm{Bax2\_Bcl2}$	
31	re32		$\mathrm{Bcl2} + \mathrm{Bax4} \rightleftharpoons \mathrm{Bax4\_Bcl2}$	
32	re33		$\mathrm{Bax4} + \mathrm{M} \rightleftharpoons \mathrm{Bax4\_M}$	
33	re34		$\mathrm{Bax4\_M} \longrightarrow \mathrm{M\_hash}$	
34	re35		$\mathrm{M\_hash} + \mathrm{Smacm} \rightleftharpoons \mathrm{M\_hash\_Smacm}$	
35	re36		$\mathrm{M\_hash\_Smacm} \longrightarrow \mathrm{M\_hash} + \mathrm{Smacr}$	
36	re37		$\mathrm{Smacr} \rightleftharpoons \mathrm{Smac}$	
37	re38		$\mathrm{M\_hash} + \mathrm{CytoCm} \rightleftharpoons \mathrm{M\_hash\_CytoCm}$	
38	re39		$\mathrm{M\_hash\_CytoCm} \longrightarrow \mathrm{CytoCr} + \mathrm{M\_hash}$	
39	re40		$\mathrm{CytoCr} \rightleftharpoons \mathrm{CytoC}$	
40	re41		$\mathrm{CytoC} + \mathrm{Apaf} \rightleftharpoons \mathrm{CytoC\_Apaf}$	
41	re42		$\mathrm{CytoC\_Apaf} \longrightarrow \mathrm{CytoC} + \mathrm{Apaf\_hash}$	
42	re43		$\mathrm{Apaf\_hash} + \mathrm{pC9} \rightleftharpoons \mathrm{Apop}$	

7.1 Reaction re1

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{L} + \mathrm{R} \rightleftharpoons \mathrm{L\_R} \tag{7}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
L	L	
R	R	

Product

Table 7: Properties of each product.

Id	Name	SBO
L_R	L:R	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{L}] \cdot [\mathrm{R}] \cdot \mathrm{k1} - [\mathrm{L\_R}] \cdot \mathrm{k\_1}) \tag{8}$$

7.2 Reaction re2

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

Reaction equation

$$\mathrm{L\_R} \longrightarrow \mathrm{R\_hash} \tag{9}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
L_R	L:R	

Product

Table 9: Properties of each product.

Id	Name	SBO
R_hash	R#	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{L\_R}] \cdot \mathrm{kc1} \tag{10}$$

7.3 Reaction re3

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{R\_hash} + \mathrm{flip} \rightleftharpoons \mathrm{flip\_R\_hash} \tag{11}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
R_hash	R#	
flip	flip	

Product

Table 11: Properties of each product.

Id	Name	SBO
flip_R_hash	flip:R#	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{R\_hash}] \cdot [\mathrm{flip}] \cdot \mathrm{k2} - [\mathrm{flip\_R\_hash}] \cdot \mathrm{k\_2}) \tag{12}$$

7.4 Reaction re4

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{R\_hash} + \mathrm{pC8} \rightleftharpoons \mathrm{R\_hash\_pC8} \tag{13}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
R_hash	R#	
pC8	proC8	

Product

Table 13: Properties of each product.

Id	Name	SBO
R_hash_pC8	R#:pC8	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{R\_hash}] \cdot [\mathrm{pC8}] \cdot \mathrm{k3} - [\mathrm{R\_hash\_pC8}] \cdot \mathrm{k\_3}) \tag{14}$$

7.5 Reaction re5

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

Reaction equation

$$\mathrm{R\_hash\_pC8} \longrightarrow \mathrm{C8} + \mathrm{R\_hash} \tag{15}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
R_hash_pC8	R#:pC8	

Products

Table 15: Properties of each product.

Id	Name	SBO
C8	casp8	
R_hash	R#	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{R\_hash\_pC8}] \cdot \mathrm{kc3} \tag{16}$$

7.6 Reaction re6

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{C6} + \mathrm{pC8} \rightleftharpoons \mathrm{C6\_pC8} \tag{17}$$

Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
C6	casp6	
pC8	proC8	

Product

Table 17: Properties of each product.

Id	Name	SBO
C6_pC8	C6:pC8	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{C6}] \cdot [\mathrm{pC8}] \cdot \mathrm{k7} - [\mathrm{C6\_pC8}] \cdot \mathrm{k\_7}) \tag{18}$$

7.7 Reaction re7

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

Reaction equation

$$\mathrm{C6\_pC8} \longrightarrow \mathrm{C8} + \mathrm{C6} \tag{19}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
C6_pC8	C6:pC8	

Products

Table 19: Properties of each product.

Id	Name	SBO
C8	casp8	
C6	casp6	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{C6\_pC8}] \cdot \mathrm{kc7} \tag{20}$$

7.8 Reaction re8

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{C8} + \mathrm{BAR} \rightleftharpoons \mathrm{BAR\_C8} \tag{21}$$

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
C8	casp8	

Id	Name	SBO
BAR	BAR	

Product

Table 21: Properties of each product.

Id	Name	SBO
BAR_C8	BAR:C8	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{C8}] \cdot [\mathrm{BAR}] \cdot \mathrm{k4} - [\mathrm{BAR\_C8}] \cdot \mathrm{k\_4}) \tag{22}$$

7.9 Reaction re9

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{pC3} + \mathrm{C8} \rightleftharpoons \mathrm{C8\_pC3} \tag{23}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
pC3	proC3	
C8	casp8	

Product

Table 23: Properties of each product.

Id	Name	SBO
C8_pC3	C8:pC3	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{pC3}] \cdot [\mathrm{C8}] \cdot \mathrm{k5} - [\mathrm{C8\_pC3}] \cdot \mathrm{k\_5}) \tag{24}$$

7.10 Reaction `re10`

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

Reaction equation

$$\mathrm{C8\_pC3} \longrightarrow \mathrm{C8} + \mathrm{C3} \tag{25}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
`C8_pC3`	C8:pC3	

Products

Table 25: Properties of each product.

Id	Name	SBO
`C8`	casp8	
`C3`	casp3	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{C8\_pC3}] \cdot \mathrm{kc5} \tag{26}$$

7.11 Reaction `re11`

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{C8} + \mathrm{Bid} \rightleftharpoons \mathrm{C8\_Bid} \tag{27}$$

Reactants

Table 26: Properties of each reactant.

Id	Name	SBO
C8	casp8	
Bid	Bid	

Product

Table 27: Properties of each product.

Id	Name	SBO
C8_Bid	C8:Bid	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{C8}] \cdot [\mathrm{Bid}] \cdot \mathrm{k10} - [\mathrm{C8\_Bid}] \cdot \mathrm{k\_10}) \tag{28}$$

7.12 Reaction re12

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

Reaction equation

$$\mathrm{C8\_Bid} \longrightarrow \mathrm{tBid} + \mathrm{C8} \tag{29}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
C8_Bid	C8:Bid	

Products

Table 29: Properties of each product.

Id	Name	SBO
tBid	tBid	
C8	casp8	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{C8\_Bid}] \cdot \mathrm{kc10} \tag{30}$$

7.13 Reaction re13

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{pC3} + \mathrm{Apop} \rightleftharpoons \mathrm{pC3\_Apop} \tag{31}$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
pC3	proC3	
Apop	Apop	

Product

Table 31: Properties of each product.

Id	Name	SBO
pC3_Apop	pC3:Apop	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{pC3}] \cdot [\mathrm{Apop}] \cdot \mathrm{k25} - [\mathrm{pC3\_Apop}] \cdot \mathrm{k\_25}) \tag{32}$$

7.14 Reaction re14

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

Reaction equation

$$\mathrm{pC3\_Apop} \longrightarrow \mathrm{C3} + \mathrm{Apop} \tag{33}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
pC3_Apop	pC3:Apop	

Products

Table 33: Properties of each product.

Id	Name	SBO
C3	casp3	
Apop	Apop	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{pC3\_Apop}] \cdot \mathrm{kc25} \tag{34}$$

7.15 Reaction re15

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{C3} + \mathrm{pC6} \rightleftharpoons \mathrm{C3\_pC6} \tag{35}$$

Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
C3	casp3	

Id	Name	SBO
pC6	proC6	

Product

Table 35: Properties of each product.

Id	Name	SBO
C3_pC6	C3:pC6	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}(\mathrm{cell}) \cdot ([\mathrm{C3}] \cdot [\mathrm{pC6}] \cdot \mathrm{k6} - [\mathrm{C3\_pC6}] \cdot \mathrm{k\_6}) \tag{36}$$

7.16 Reaction re16

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

Reaction equation

$$\mathrm{C3\_pC6} \longrightarrow \mathrm{C3} + \mathrm{C6} \tag{37}$$

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
C3_pC6	C3:pC6	

Products

Table 37: Properties of each product.

Id	Name	SBO
C3	casp3	
C6	casp6	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{C3\_pC6}] \cdot \mathrm{kc6} \tag{38}$$

7.17 Reaction `re17`

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP} \rightleftharpoons \mathrm{XIAP\_C3} \tag{39}$$

Reactants

Table 38: Properties of each reactant.

Id	Name	SBO
`C3`	casp3	
`XIAP`	XIAP	

Product

Table 39: Properties of each product.

Id	Name	SBO
`XIAP_C3`	XIAP:C3	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{C3}] \cdot [\mathrm{XIAP}] \cdot \mathrm{k8} - [\mathrm{XIAP\_C3}] \cdot \mathrm{k\_8}) \tag{40}$$

7.18 Reaction `re18`

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

Reaction equation

$$\mathrm{XIAP\_C3} \longrightarrow \mathrm{C3\_Ub} + \mathrm{XIAP} \tag{41}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
XIAP_C3	XIAP:C3	

Products

Table 41: Properties of each product.

Id	Name	SBO
C3_Ub	Ub C3	
XIAP	XIAP	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{XIAP\_C3}] \cdot \mathrm{kc8} \tag{42}$$

7.19 Reaction re19

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{PARP} + \mathrm{C3} \rightleftharpoons \mathrm{PARP\_C3} \tag{43}$$

Reactants

Table 42: Properties of each reactant.

Id	Name	SBO
PARP	PARP	
C3	casp3	

Product

Table 43: Properties of each product.

Id	Name	SBO
PARP_C3	PARP:C3	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{PARP}] \cdot [\mathrm{C3}] \cdot \mathrm{k9} - [\mathrm{PARP\_C3}] \cdot \mathrm{k\_9}) \tag{44}$$

7.20 Reaction re20

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

Reaction equation

$$\mathrm{PARP\_C3} \longrightarrow \mathrm{CPARP} + \mathrm{C3} \tag{45}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
PARP_C3	PARP:C3	

Products

Table 45: Properties of each product.

Id	Name	SBO
CPARP	cPARP	
C3	casp3	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{PARP\_C3}] \cdot \mathrm{kc9} \tag{46}$$

7.21 Reaction re21

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{XIAP} + \mathrm{Apop} \rightleftharpoons \mathrm{Apop\_XIAP} \tag{47}$$

Reactants

Table 46: Properties of each reactant.

Id	Name	SBO
XIAP	XIAP	
Apop	Apop	

Product

Table 47: Properties of each product.

Id	Name	SBO
Apop_XIAP	Apop:XIAP	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{XIAP}] \cdot [\mathrm{Apop}] \cdot \mathrm{k27} - [\mathrm{Apop\_XIAP}] \cdot \mathrm{k\_27}) \tag{48}$$

7.22 Reaction re22

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{XIAP} + \mathrm{Smac} \rightleftharpoons \mathrm{Smac\_XIAP} \tag{49}$$

Reactants

Table 48: Properties of each reactant.

Id	Name	SBO
XIAP	XIAP	
Smac	Smac	

Product

Table 49: Properties of each product.

Id	Name	SBO
Smac_XIAP	Smac:XIAP	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{XIAP}] \cdot [\mathrm{Smac}] \cdot \mathrm{k28} - [\mathrm{Smac\_XIAP}] \cdot \mathrm{k\_28}) \tag{50}$$

7.23 Reaction re23

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{tBid} + \mathrm{Bcl2c} \rightleftharpoons \mathrm{Bcl2c\_tBid} \tag{51}$$

Reactants

Table 50: Properties of each reactant.

Id	Name	SBO
tBid	tBid	
Bcl2c	cytosolic Bcl-2	

Product

Table 51: Properties of each product.

Id	Name	SBO
Bcl2c_tBid	Bcl2c:tBid	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{tBid}] \cdot [\mathrm{Bcl2c}] \cdot \mathrm{k11} - [\mathrm{Bcl2c\_tBid}] \cdot \mathrm{k\_11}) \tag{52}$$

7.24 Reaction re24

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{tBid} + \mathrm{Bax} \rightleftharpoons \mathrm{Bax\_tBid} \tag{53}$$

Reactants

Table 52: Properties of each reactant.

Id	Name	SBO
tBid	tBid	
Bax	Bax	

Product

Table 53: Properties of each product.

Id	Name	SBO
Bax_tBid	Bax:tBid	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{tBid}] \cdot [\mathrm{Bax}] \cdot \mathrm{k12} - [\mathrm{Bax\_tBid}] \cdot \mathrm{k\_12}) \tag{54}$$

7.25 Reaction re25

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

Reaction equation

$$\mathrm{Bax\_tBid} \longrightarrow \mathrm{tBid} + \mathrm{Bax\_hash} \tag{55}$$

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
Bax_tBid	Bax:tBid	

Products

Table 55: Properties of each product.

Id	Name	SBO
tBid	tBid	
Bax_hash	Bax#	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{Bax\_tBid}] \cdot \mathrm{kc12} \tag{56}$$

7.26 Reaction re26

This is a reversible reaction of one reactant forming one product.

Reaction equation

$$\mathrm{Bax\_hash} \rightleftharpoons \mathrm{Baxm} \tag{57}$$

Reactant

Table 56: Properties of each reactant.

Id	Name	SBO
Bax_hash	Bax#	

Product

Table 57: Properties of each product.

Id	Name	SBO
Baxm	Baxm	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{Bax\_hash}] \cdot \mathrm{k13} - [\mathrm{Baxm}] \cdot \mathrm{k\_13}) \tag{58}$$

7.27 Reaction re27

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{Baxm} + \mathrm{Bcl2} \rightleftharpoons \mathrm{Baxm\_Bcl2} \tag{59}$$

Reactants

Table 58: Properties of each reactant.

Id	Name	SBO
Baxm	Baxm	
Bcl2	Bcl-2	

Product

Table 59: Properties of each product.

Id	Name	SBO
Baxm_Bcl2	Baxm:Bcl2	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \left(\frac{[\mathrm{Baxm}] \cdot [\mathrm{Bcl2}] \cdot \mathrm{k14}}{\mathrm{v}} - [\mathrm{Baxm\_Bcl2}] \cdot \mathrm{k\_14} \right) \tag{60}$$

7.28 Reaction re29

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{Baxm} + \mathrm{Baxm} \rightleftharpoons \mathrm{Bax2} \tag{61}$$

Reactants

Table 60: Properties of each reactant.

Id	Name	SBO
Baxm	Baxm	
Baxm	Baxm	

Product

Table 61: Properties of each product.

Id	Name	SBO
Bax2	Bax2	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \left(\frac{[\mathrm{Baxm}] \cdot [\mathrm{Baxm}] \cdot \mathrm{k15}}{\mathrm{v}} - [\mathrm{Bax2}] \cdot \mathrm{k\_15} \right) \tag{62}$$

7.29 Reaction re30

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{Bax2} + \mathrm{Bax2} \rightleftharpoons \mathrm{Bax4} \tag{63}$$

Reactants

Table 62: Properties of each reactant.

Id	Name	SBO
Bax2	Bax2	
Bax2	Bax2	

Product

Table 63: Properties of each product.

Id	Name	SBO
Bax4	Bax4	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \left(\frac{[\mathrm{Bax2}] \cdot [\mathrm{Bax2}] \cdot \mathrm{k17}}{\mathrm{v}} - [\mathrm{Bax4}] \cdot \mathrm{k\_17} \right) \tag{64}$$

7.30 Reaction re31

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{Bcl2} + \mathrm{Bax2} \rightleftharpoons \mathrm{Bax2\_Bcl2} \tag{65}$$

Reactants

Table 64: Properties of each reactant.

Id	Name	SBO
Bcl2	Bcl-2	
Bax2	Bax2	

Product

Table 65: Properties of each product.

Id	Name	SBO
Bax2_Bcl2	Bax2:Bcl2	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \left(\frac{[\mathrm{Bcl2}] \cdot [\mathrm{Bax2}] \cdot \mathrm{k16}}{\mathrm{v}} - [\mathrm{Bax2\_Bcl2}] \cdot \mathrm{k\_16} \right) \tag{66}$$

7.31 Reaction re32

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{Bcl2} + \mathrm{Bax4} \rightleftharpoons \mathrm{Bax4\_Bcl2} \tag{67}$$

Reactants

Table 66: Properties of each reactant.

Id	Name	SBO
Bcl2	Bcl-2	
Bax4	Bax4	

Product

Table 67: Properties of each product.

Id	Name	SBO
Bax4_Bcl2	Bax4:Bcl2	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \left(\frac{[\mathrm{Bcl2}] \cdot [\mathrm{Bax4}] \cdot \mathrm{k18}}{\mathrm{v}} - [\mathrm{Bax4\_Bcl2}] \cdot \mathrm{k\_18} \right) \tag{68}$$

7.32 Reaction re33

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{Bax4} + \mathrm{M} \rightleftharpoons \mathrm{Bax4\_M} \tag{69}$$

Reactants

Table 68: Properties of each reactant.

Id	Name	SBO
Bax4	Bax4	
M	M	

Product

Table 69: Properties of each product.

Id	Name	SBO
Bax4_M	Bax4:M	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \left(\frac{[\mathrm{Bax4}] \cdot [\mathrm{M}] \cdot \mathrm{k19}}{\mathrm{v}} - [\mathrm{Bax4\_M}] \cdot \mathrm{k\_19} \right) \tag{70}$$

7.33 Reaction re34

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

Reaction equation

$$\mathrm{Bax4\_M} \longrightarrow \mathrm{M\_hash} \tag{71}$$

Reactant

Table 70: Properties of each reactant.

Id	Name	SBO
Bax4_M	Bax4:M	

Product

Table 71: Properties of each product.

Id	Name	SBO
M_hash	M#	

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot [\mathrm{Bax4\_M}] \cdot \mathrm{kc19} \tag{72}$$

7.34 Reaction `re35`

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{M\_hash} + \mathrm{Smacm} \rightleftharpoons \mathrm{M\_hash\_Smacm} \tag{73}$$

Reactants

Table 72: Properties of each reactant.

Id	Name	SBO
`M_hash`	M#	
`Smacm`	Smac_m	

Product

Table 73: Properties of each product.

Id	Name	SBO
`M_hash_Smacm`	M#:Smac_m	

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \left(\frac{[\mathrm{M\_hash}] \cdot [\mathrm{Smacm}] \cdot \mathrm{k21}}{\mathrm{v}} - [\mathrm{M\_hash\_Smacm}] \cdot \mathrm{k\_21} \right) \tag{74}$$

7.35 Reaction `re36`

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

Reaction equation

$$\mathrm{M\_hash\_Smacm} \longrightarrow \mathrm{M\_hash} + \mathrm{Smacr} \tag{75}$$

Reactant

Table 74: Properties of each reactant.

Id	Name	SBO
M_hash_Smacm	M#:Smac_m	

Products

Table 75: Properties of each product.

Id	Name	SBO
M_hash	M#	
Smacr	Smac released	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot [\mathrm{M\_hash\_Smacm}] \cdot \mathrm{kc21} \tag{76}$$

7.36 Reaction re37

This is a reversible reaction of one reactant forming one product.

Reaction equation

$$\mathrm{Smacr} \rightleftharpoons \mathrm{Smac} \tag{77}$$

Reactant

Table 76: Properties of each reactant.

Id	Name	SBO
Smacr	Smac released	

Product

Table 77: Properties of each product.

Id	Name	SBO
Smac	Smac	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{Smacr}] \cdot \mathrm{k26} - [\mathrm{Smac}] \cdot \mathrm{k\_26}) \tag{78}$$

7.37 Reaction re38

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{M\_hash} + \mathrm{CytoCm} \rightleftharpoons \mathrm{M\_hash\_CytoCm} \tag{79}$$

Reactants

Table 78: Properties of each reactant.

Id	Name	SBO
M_hash	M#	
CytoCm	CytoC_m	

Product

Table 79: Properties of each product.

Id	Name	SBO
M_hash_CytoCm	M#:CytoC_m	

Kinetic Law

Derived unit contains undeclared units

$$v_{37} = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \left(\frac{[\mathrm{M\_hash}] \cdot [\mathrm{CytoCm}] \cdot \mathrm{k20}}{\mathrm{v}} - [\mathrm{M\_hash\_CytoCm}] \cdot \mathrm{k\_20} \right) \tag{80}$$

7.38 Reaction re39

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

Reaction equation

$$\text{M\_hash\_CytoCm} \longrightarrow \text{CytoCr} + \text{M\_hash} \tag{81}$$

Reactant

Table 80: Properties of each reactant.

Id	Name	SBO
M_hash_CytoCm	M#:CytoC_m	

Products

Table 81: Properties of each product.

Id	Name	SBO
CytoCr	CytoC released	
M_hash	M#	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \text{vol}\left(\text{mitochondrion}\right) \cdot [\text{M\_hash\_CytoCm}] \cdot \text{kc20} \tag{82}$$

7.39 Reaction re40

This is a reversible reaction of one reactant forming one product.

Reaction equation

$$\text{CytoCr} \rightleftharpoons \text{CytoC} \tag{83}$$

Reactant

Table 82: Properties of each reactant.

Id	Name	SBO
CytoCr	CytoC released	

Product

Table 83: Properties of each product.

Id	Name	SBO
CytoC	CytoC	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{CytoCr}] \cdot \mathrm{k22} - [\mathrm{CytoC}] \cdot \mathrm{k\_22}) \tag{84}$$

7.40 Reaction re41

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{CytoC} + \mathrm{Apaf} \rightleftharpoons \mathrm{CytoC\_Apaf} \tag{85}$$

Reactants

Table 84: Properties of each reactant.

Id	Name	SBO
CytoC	CytoC	
Apaf	Apaf	

Product

Table 85: Properties of each product.

Id	Name	SBO
CytoC_Apaf	CytoC:Apaf	

Kinetic Law

Derived unit contains undeclared units

$$v_{40} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{CytoC}] \cdot [\mathrm{Apaf}] \cdot \mathrm{k23} - [\mathrm{CytoC\_Apaf}] \cdot \mathrm{k\_23}) \tag{86}$$

7.41 Reaction re42

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

Reaction equation

$$\text{CytoC\_Apaf} \longrightarrow \text{CytoC} + \text{Apaf\_hash} \tag{87}$$

Reactant

Table 86: Properties of each reactant.

Id	Name	SBO
CytoC_Apaf	CytoC:Apaf	

Products

Table 87: Properties of each product.

Id	Name	SBO
CytoC	CytoC	
Apaf_hash	Apaf#	

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = \text{vol}(\text{cell}) \cdot [\text{CytoC\_Apaf}] \cdot \text{kc23} \tag{88}$$

7.42 Reaction re43

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\text{Apaf\_hash} + \text{pC9} \rightleftharpoons \text{Apop} \tag{89}$$

Reactants

Table 88: Properties of each reactant.

Id	Name	SBO
Apaf_hash	Apaf#	

Id	Name	SBO
pC9	proC9	

Product

Table 89: Properties of each product.

Id	Name	SBO
Apop	Apop	

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{Apaf\_hash}] \cdot [\mathrm{pC9}] \cdot \mathrm{k24} - [\mathrm{Apop}] \cdot \mathrm{k\_24}) \tag{90}$$

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 L

Name L

Notes **TRAIL** : L = 3000 correspond to 50 ng/ml SuperKiller TRAIL
for experiments under saturating conditions use L = 60000

Initial amount 3000 mol

Charge 0

This species takes part in one reaction (as a reactant in re1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{L} = -v_1 \tag{91}$$

8.2 Species R

Name R

Notes **TRAIL receptor** : for experiments without siRNA R = 200

Initial amount 200 mol

Charge 0

This species takes part in one reaction (as a reactant in re1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R} = -v_1 \tag{92}$$

8.3 Species flip

Name flip

Initial amount 100 mol

Charge 0

This species takes part in one reaction (as a reactant in re3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{flip} = -v_3 \tag{93}$$

8.4 Species pC8

Name proC8

Initial amount 20000 mol

Charge 0

This species takes part in two reactions (as a reactant in re4, re6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{pC8} = -v_4 - v_6 \tag{94}$$

8.5 Species C8

Name casp8

Initial amount 0 mol

Charge 0

This species takes part in seven reactions (as a reactant in re8, re9, re11 and as a product in re5, re7, re10, re12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C8} = v_5 + v_7 + v_{10} + v_{12} - v_8 - v_9 - v_{11} \tag{95}$$

8.6 Species C6

Name casp6

Initial amount 0 mol

Charge 0

This species takes part in three reactions (as a reactant in re6 and as a product in re7, re16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C6} = v_7 + v_{16} - v_6 \tag{96}$$

8.7 Species BAR

Name BAR

Initial amount 1000 mol

Charge 0

This species takes part in one reaction (as a reactant in re8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BAR} = -v_8 \tag{97}$$

8.8 Species pC3

Name proC3

Initial amount 10000 mol

Charge 0

This species takes part in two reactions (as a reactant in re9, re13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{pC3} = -v_9 - v_{13} \tag{98}$$

8.9 Species C3

Name casp3

Initial amount 0 mol

Charge 0

This species takes part in seven reactions (as a reactant in re15, re17, re19 and as a product in re10, re14, re16, re20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C3} = v_{10} + v_{14} + v_{16} + v_{20} - v_{15} - v_{17} - v_{19} \tag{99}$$

8.10 Species Bid

Name Bid

Initial amount 40000 mol

Charge 0

This species takes part in one reaction (as a reactant in re11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bid} = -v_{11} \tag{100}$$

8.11 Species tBid

Name tBid

Initial amount 0 mol

Charge 0

This species takes part in four reactions (as a reactant in re23, re24 and as a product in re12, re25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{tBid} = v_{12} + v_{25} - v_{23} - v_{24} \tag{101}$$

8.12 Species pC6

Name proC6

Initial amount 10000 mol

Charge 0

This species takes part in one reaction (as a reactant in re15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{pC6} = -v_{15} \tag{102}$$

8.13 Species XIAP

Name XIAP

Initial amount 100000 mol

Charge 0

This species takes part in four reactions (as a reactant in re17, re21, re22 and as a product in re18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{XIAP} = v_{18} - v_{17} - v_{21} - v_{22} \tag{103}$$

8.14 Species C3_Ub

Name Ub C3

Notes ubiquitinylated caspase 3

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C3\_Ub} = v_{18} \tag{104}$$

8.15 Species PARP

Name PARP

Notes EC substrate

Initial amount 1000000 mol

Charge 0

This species takes part in one reaction (as a reactant in re19).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PARP} = -v_{19} \tag{105}$$

8.16 Species CPARP

Name cPARP

Notes cleaved PARP

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CPARP} = v_{20} \tag{106}$$

8.17 Species Smac

Name Smac

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re22 and as a product in re37).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Smac} = v_{36} - v_{22} \tag{107}$$

8.18 Species Bcl2c

Name cytosolic Bcl-2

Initial amount 20000 mol

Charge 0

This species takes part in one reaction (as a reactant in re23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bcl2c} = -v_{23} \tag{108}$$

8.19 Species Bax

Name Bax

Initial amount 100000 mol

Charge 0

This species takes part in one reaction (as a reactant in re24).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bax} = -v_{24} \tag{109}$$

8.20 Species Bax_hash

Name Bax#

Notes activated Bax

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re26 and as a product in re25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bax\_hash} = v_{25} - v_{26} \tag{110}$$

8.21 Species Bcl2

Name Bcl-2

Notes mitochondrial Bcl-2

Initial amount 20000 mol

Charge 0

This species takes part in three reactions (as a reactant in re27, re31, re32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bcl2} = -v_{27} - v_{30} - v_{31} \tag{111}$$

8.22 Species L_R

Name L:R

Notes TRAIL-receptor complex

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re2 and as a product in re1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{L\_R} = v_1 - v_2 \tag{112}$$

8.23 Species R_hash

Name R#

Notes activated receptor

Initial amount 0 mol

Charge 0

This species takes part in four reactions (as a reactant in re3, re4 and as a product in re2, re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R\_hash} = v_2 + v_5 - v_3 - v_4 \tag{113}$$

8.24 Species flip_R_hash

Name flip:R#

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{flip\_R\_hash} = v_3 \tag{114}$$

8.25 Species R_hash_pC8

Name R#:pC8

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re5 and as a product in re4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R\_hash\_pC8} = v_4 - v_5 \tag{115}$$

8.26 Species C6_pC8

Name C6:pC8

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re7 and as a product in re6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C6\_pC8} = v_6 - v_7 \tag{116}$$

8.27 Species BAR_C8

Name BAR:C8

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BAR\_C8} = v_8 \tag{117}$$

8.28 Species C8_pC3

Name C8:pC3

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re10 and as a product in re9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C8\_pC3} = v_9 - v_{10} \tag{118}$$

8.29 Species pC3_Apop

Name pC3:Apop

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re14 and as a product in re13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{pC3\_Apop} = v_{13} - v_{14} \tag{119}$$

8.30 Species Apop

Name Apop

Notes apoptosome

Initial amount 0 mol

Charge 0

This species takes part in four reactions (as a reactant in re13, re21 and as a product in re14, re43).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Apop} = v_{14} + v_{42} - v_{13} - v_{21} \tag{120}$$

8.31 Species C8_Bid

Name C8:Bid

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re12 and as a product in re11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C8\_Bid} = v_{11} - v_{12} \tag{121}$$

8.32 Species C3_pC6

Name C3:pC6

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re16 and as a product in re15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C3\_pC6} = v_{15} - v_{16} \tag{122}$$

8.33 Species XIAP_C3

Name XIAP:C3

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re18 and as a product in re17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{XIAP\_C3} = v_{17} - v_{18} \tag{123}$$

8.34 Species PARP_C3

Name PARP:C3

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re20 and as a product in re19).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PARP\_C3} = v_{19} - v_{20} \tag{124}$$

8.35 Species Apop_XIAP

Name Apop:XIAP

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re21).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Apop\_XIAP} = v_{21} \tag{125}$$

8.36 Species Smac_XIAP

Name Smac:XIAP

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re22).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Smac\_XIAP} = v_{22} \tag{126}$$

8.37 Species Bcl2c_tBid

Name Bcl2c:tBid

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bcl2c\_tBid} = v_{23} \tag{127}$$

8.38 Species Bax_tBid

Name Bax:tBid

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re25 and as a product in re24).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bax\_tBid} = v_{24} - v_{25} \tag{128}$$

8.39 Species Baxm_Bcl2

Name Baxm:Bcl2

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re27).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Baxm\_Bcl2} = v_{27} \tag{129}$$

8.40 Species Bax4

Name Bax4

Notes Bax tetramer

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re32, re33 and as a product in re30).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bax4} = v_{29} - v_{31} - v_{32} \tag{130}$$

8.41 Species Bax2_Bcl2

Name Bax2:Bcl2

Initial amount 0 mol

This species takes part in one reaction (as a product in re31).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bax2\_Bcl2} = v_{30} \tag{131}$$

8.42 Species Bax4_Bcl2

Name Bax4:Bcl2

Initial amount 0 mol

This species takes part in one reaction (as a product in re32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bax4\_Bcl2} = v_{31} \tag{132}$$

8.43 Species M

Name M

Notes binding sites for activated Bax on the inner mitochondrial membrane

Initial amount 500000 mol

Charge 0

This species takes part in one reaction (as a reactant in re33).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M} = -v_{32} \tag{133}$$

8.44 Species Bax4_M

Name Bax4:M

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re34 and as a product in re33).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bax4\_M} = v_{32} - v_{33} \tag{134}$$

8.45 Species M_hash

Name M#

Notes opened inner mitochondrial membrane pore

Initial amount 0 mol

This species takes part in five reactions (as a reactant in re35, re38 and as a product in re34, re36, re39).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M\_hash} = v_{33} + v_{35} + v_{38} - v_{34} - v_{37} \tag{135}$$

8.46 Species Smacm

Name Smac_m

Initial amount 100000 mol

Charge 0

This species takes part in one reaction (as a reactant in re35).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Smacm} = -v_{34} \tag{136}$$

8.47 Species M_hash_Smacm

Name M#:Smac_m

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re36 and as a product in re35).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M\_hash\_Smacm} = v_{34} - v_{35} \tag{137}$$

8.48 Species Smacr

Name Smac released

Notes Smac released into the mitochondrial intermembrane space

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re37 and as a product in re36).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Smacr} = v_{35} - v_{36} \tag{138}$$

8.49 Species CytoCm

Name CytoC_m

Initial amount 500000 mol

Charge 0

This species takes part in one reaction (as a reactant in re38).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CytoCm} = -v_{37} \tag{139}$$

8.50 Species M_hash_CytoCm

Name M#:CytoC_m

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re39 and as a product in re38).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M\_hash\_CytoCm} = v_{37} - v_{38} \tag{140}$$

8.51 Species CytoCr

Name CytoC released

Notes cytochrom C released into the mitochondrial intermembrane space

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re40 and as a product in re39).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CytoCr} = v_{38} - v_{39} \tag{141}$$

8.52 Species CytoC

Name CytoC

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re41 and as a product in re40, re42).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CytoC} = v_{39} + v_{41} - v_{40} \tag{142}$$

8.53 Species Apaf

Name Apaf

Initial amount 100000 mol

Charge 0

This species takes part in one reaction (as a reactant in re41).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Apaf} = -v_{40} \tag{143}$$

8.54 Species CytoC_Apaf

Name CytoC:Apaf

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re42 and as a product in re41).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CytoC\_Apaf} = v_{40} - v_{41} \tag{144}$$

8.55 Species Apaf_hash

Name Apaf#

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re43 and as a product in re42).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Apaf\_hash} = v_{41} - v_{42} \tag{145}$$

8.56 Species pC9

Name proC9

Initial amount 100000 mol

Charge 0

This species takes part in one reaction (as a reactant in re43).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{pC9} = -v_{42} \tag{146}$$

8.57 Species Baxm

Name Baxm

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re27, re29, re29 and as a product in re26).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Baxm} = v_{26} - v_{27} - v_{28} - v_{28} \tag{147}$$

8.58 Species Bax2

Name Bax2

Notes dimeric Bax

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re30, re30, re31 and as a product in re29).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bax2} = v_{28} - v_{29} - v_{29} - v_{30} \tag{148}$$

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