SBML Model Report

Model name: “Legewie2006_apoptosis_WT”

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following four authors: Harish Dharuri[1], Stefan Legewie[2], Nils Bluethgen[3] and Hanspeter Herzel[4] at April 20th 2006 at 10:59 a. m. and last time modified at March fifth 2014 at 4:59 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	1
species types	0	species	13
events	0	constraints	0
reactions	28	function definitions	0
global parameters	41	unit definitions	5
rules	0	initial assignments	0

Model Notes

The model reproduces active Caspase-3 time profile corresponding to the total Apaf-1 value of 20 nM as depicted in Fig 2-A . The model was successfully tested on MathSBML.

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2 Unit Definitions

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

2.1 Unit `substance`

Name nanomole

Definition nmol

2.2 Unit `nM_per_sec`

Name nM_per_sec

Definition $\mathrm{nmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$

2.3 Unit `per_nM_per_sec`

Name per_nM_per_sec

Definition $\mathrm{nmol}^{-1} \cdot \mathrm{l} \cdot \mathrm{s}^{-1}$

2.4 Unit `nM`

Name nM

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

2.5 Unit `sec_inverse`

Name sec_inverse

Definition s^{-1}

2.6 Unit `volume`

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

Definition l

2.7 Unit `area`

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

Definition m^2

2.8 Unit `length`

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

Definition m

2.9 Unit `time`

Notes Second is the predefined SBML unit for `time`.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`cytosol`	Cytosol		3	1	litre	☑	

3.1 Compartment `cytosol`

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

Name Cytosol

4 Species

This model contains 13 species. Section 7 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
A	APAF-1	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C9	Caspase 9	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C9X	Caspase 9-XIAP complex	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X	XIAP	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
AC9X	APAF-1-Caspase 9-XIAP complex	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
AC9	APAF-1-Caspase 9 complex	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C3	Caspase 3	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C3_star	Caspase 3 cleaved	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C3_starX	Caspase 3 cleaved - XIAP complex	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C9_starX	Caspase 9 cleaved-XIAP complex	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C9_star	Caspase 9 cleaved	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
AC9_star	APAF-1-Caspase 9 cleaved complex	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
AC9_starX	Apaf-1-Caspase 9 cleaved -XIAP complex	cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 41 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.002	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
kb1			0.100	s^{-1}	☑
k2			$5 \cdot 10^{-6}$	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k3			$3.5 \cdot 10^{-4}$	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k4			$2 \cdot 10^{-4}$	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k5			$2 \cdot 10^{-4}$	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k6			$5 \cdot 10^{-5}$	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k7			0.004	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k8			0.002	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k8b			0.100	s^{-1}	☑
k9			0.001	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k9b			0.001	s^{-1}	☑
k10			0.001	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k10b			0.001	s^{-1}	☑
k11			0.001	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k11b			0.001	s^{-1}	☑
k12			0.001	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k12b			0.001	s^{-1}	☑
k13			0.002	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k13b			0.100	s^{-1}	☑
k14			0.002	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k14b			0.100	s^{-1}	☑
k15			0.003	$\mathrm{nmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k15b			0.001	s^{-1}	☑
k16			0.001	s^{-1}	☑
k16prod			0.020	$\mathrm{nmol} \cdot 1^{-1} \cdot \mathrm{s}^{-1}$	☑
k17			0.001	s^{-1}	☑
k17prod			0.020	$\mathrm{nmol} \cdot 1^{-1} \cdot \mathrm{s}^{-1}$	☑
k18			0.001	s^{-1}	☑
k18prod			0.040	$\mathrm{nmol} \cdot 1^{-1} \cdot \mathrm{s}^{-1}$	☑
k19			0.001	s^{-1}	☑
k20			0.001	s^{-1}	☑
k21			0.001	s^{-1}	☑
k22			0.001	s^{-1}	☑
k22prod			0.200	$\mathrm{nmol} \cdot 1^{-1} \cdot \mathrm{s}^{-1}$	☑
k23			0.001	s^{-1}	☑

Id	Name	SBO	Value	Unit	Constant
k24			0.001	s^{-1}	☑
k25			0.001	s^{-1}	☑
k26			0.001	s^{-1}	☑
k27			0.001	s^{-1}	☑
k28			0.001	s^{-1}	☑

6 Reactions

This model contains 28 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	v1	Caspase 9 / Apaf-1 binding	$A + C9 \rightleftharpoons AC9$	
2	v2	Caspase 3 cleavage by Caspase 9	$C3 + C9 \longrightarrow C3\_star + C9$	
3	v3	Caspase 3 cleavage by Caspase 9-Apaf-1	$C3 + AC9 \longrightarrow C3\_star + AC9$	
4	v9	Caspase 9 Xiap binding	$C9 + X \rightleftharpoons C9X$	
5	v10	Caspase 9-Apaf-1 Xiap binding	$AC9 + X \rightleftharpoons AC9X$	
6	v13	Caspase 9-Xiap Apaf-1 binding	$C9X + A \rightleftharpoons AC9X$	
7	v15	cleaved Caspase 3-Xiap binding	$C3\_star + X \rightleftharpoons C3\_starX$	
8	v4	Caspase 9 cleavage by cleaved caspase 3	$C9 + C3\_star \longrightarrow C9\_star + C3\_star$	
9	v5	Caspase 9 cleavage by cleaved caspase 3 when Apaf-1 is bound	$AC9 + C3\_star \longrightarrow AC9\_star + C3\_star$	
10	v8	cleaved Caspase 9 Apaf-1 binding	$C9\_star + A \rightleftharpoons AC9\_star$	
11	v11	cleaved Caspase 9 XIAP binding	$C9\_star + X \rightleftharpoons C9\_starX$	
12	v12	cleaved Caspase 9-Apaf-1 XIAP binding	$AC9\_star + X \rightleftharpoons AC9\_starX$	
13	v14	cleaved Caspase 9-Xiap Apaf-1 binding	$C9\_starX + A \rightleftharpoons AC9\_starX$	
14	v6	Caspase 3 cleavage by cleaved Caspase 9	$C3 + C9\_star \longrightarrow C3\_star + C9\_star$	
15	v7	Caspase 3 cleavage by cleaved Caspase 9 - Apaf-1	$C3 + AC9\_star \longrightarrow C3\_star + AC9\_star$	
16	v16	Apaf-1 turnover	$\emptyset \longrightarrow A$	
17	v17	Caspase 9 turnover	$\emptyset \longrightarrow C9$	
18	v18	Xiap turnover	$\emptyset \longrightarrow X$	
19	v19	Caspase 9-Xiap degradation	$C9X \longrightarrow \emptyset$	
20	v20	Apaf-1-Caspase 9-Xiap degradation	$AC9X \longrightarrow \emptyset$	
21	v21	Apaf-1-Caspase 9 degradation	$AC9 \longrightarrow \emptyset$	

№	Id	Name	Reaction Equation	SBO
22	v22	Caspase 3 turnover	$\emptyset \longrightarrow$ C3	
23	v23	Caspase 3 cleaved degradation	C3_star $\longrightarrow \emptyset$	
24	v24	Caspase 3 cleaved-Xiap degradation	C3_starX $\longrightarrow \emptyset$	
25	v25	Caspase 9 cleaved-Xiap degradation	C9_starX $\longrightarrow \emptyset$	
26	v26	Caspase 9 cleaved degradation	C9_star $\longrightarrow \emptyset$	
27	v27	Apaf-1 Caspase 9 cleaved degradation	AC9_star $\longrightarrow \emptyset$	
28	v28	Apaf-1 Caspase 9 cleaved-Xiap degradation	AC9_starX $\longrightarrow \emptyset$	

6.1 Reaction v1

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

Name Caspase 9 / Apaf-1 binding

Reaction equation

$$\mathrm{A} + \mathrm{C9} \rightleftharpoons \mathrm{AC9} \tag{1}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
A	APAF-1	
C9	Caspase 9	

Product

Table 7: Properties of each product.

Id	Name	SBO
AC9	APAF-1-Caspase 9 complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_1 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{k1} \cdot [\mathrm{A}] \cdot [\mathrm{C9}] - \mathrm{kb1} \cdot [\mathrm{AC9}]) \tag{2}$$

6.2 Reaction v2

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

Name Caspase 3 cleavage by Caspase 9

Reaction equation

$$\mathrm{C3} + \mathrm{C9} \longrightarrow \mathrm{C3\_star} + \mathrm{C9} \tag{3}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
C3	Caspase 3	
C9	Caspase 9	

Products

Table 9: Properties of each product.

Id	Name	SBO
C3_star	Caspase 3 cleaved	
C9	Caspase 9	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_2 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k2} \cdot [\mathrm{C3}] \cdot [\mathrm{C9}] \tag{4}$$

6.3 Reaction v3

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

Name Caspase 3 cleavage by Caspase 9-Apaf-1

Reaction equation

$$\mathrm{C3} + \mathrm{AC9} \longrightarrow \mathrm{C3\_star} + \mathrm{AC9} \tag{5}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
C3	Caspase 3	
AC9	APAF-1-Caspase 9 complex	

Products

Table 11: Properties of each product.

Id	Name	SBO
C3_star	Caspase 3 cleaved	
AC9	APAF-1-Caspase 9 complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_3 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k3} \cdot [\mathrm{C3}] \cdot [\mathrm{AC9}] \tag{6}$$

6.4 Reaction v9

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

Name Caspase 9 Xiap binding

Reaction equation

$$\mathrm{C9} + \mathrm{X} \rightleftharpoons \mathrm{C9X} \tag{7}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
C9	Caspase 9	
X	XIAP	

Product

Table 13: Properties of each product.

Id	Name	SBO
C9X	Caspase 9-XIAP complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_4 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{k9} \cdot [\mathrm{C9}] \cdot [\mathrm{X}] - \mathrm{k9b} \cdot [\mathrm{C9X}]) \tag{8}$$

6.5 Reaction v10

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

Name Caspase 9-Apaf-1 Xiap binding

Reaction equation

$$\mathrm{AC9} + \mathrm{X} \rightleftharpoons \mathrm{AC9X} \tag{9}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
AC9	APAF-1-Caspase 9 complex	
X	XIAP	

Product

Table 15: Properties of each product.

Id	Name	SBO
AC9X	APAF-1-Caspase 9-XIAP complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_5 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{k10} \cdot [\mathrm{AC9}] \cdot [\mathrm{X}] - \mathrm{k10b} \cdot [\mathrm{AC9X}]) \tag{10}$$

6.6 Reaction v13

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

Name Caspase 9-Xiap Apaf-1 binding

Reaction equation

$$\mathrm{C9X} + \mathrm{A} \rightleftharpoons \mathrm{AC9X} \tag{11}$$

Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
C9X	Caspase 9-XIAP complex	
A	APAF-1	

Product

Table 17: Properties of each product.

Id	Name	SBO
AC9X	APAF-1-Caspase 9-XIAP complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_6 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{k13} \cdot [\mathrm{C9X}] \cdot [\mathrm{A}] - \mathrm{k13b} \cdot [\mathrm{AC9X}]) \tag{12}$$

6.7 Reaction v15

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

Name cleaved Caspase 3-Xiap binding

Reaction equation

$$\mathrm{C3\_star} + \mathrm{X} \rightleftharpoons \mathrm{C3\_starX} \tag{13}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
C3_star	Caspase 3 cleaved	
X	XIAP	

Product

Table 19: Properties of each product.

Id	Name	SBO
C3_starX	Caspase 3 cleaved - XIAP complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_7 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{k15} \cdot [\mathrm{C3\_star}] \cdot [\mathrm{X}] - \mathrm{k15b} \cdot [\mathrm{C3\_starX}]) \tag{14}$$

6.8 Reaction v4

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

Name Caspase 9 cleavage by cleaved caspase 3

Reaction equation

$$\mathrm{C9} + \mathrm{C3\_star} \longrightarrow \mathrm{C9\_star} + \mathrm{C3\_star} \tag{15}$$

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
C9	Caspase 9	
C3_star	Caspase 3 cleaved	

Products

Table 21: Properties of each product.

Id	Name	SBO
C9_star	Caspase 9 cleaved	
C3_star	Caspase 3 cleaved	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_8 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k4} \cdot [\mathrm{C9}] \cdot [\mathrm{C3\_star}] \tag{16}$$

6.9 Reaction v5

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

Name Caspase 9 cleavage by cleaved caspase 3 when Apaf-1 is bound

Reaction equation

$$\mathrm{AC9} + \mathrm{C3\_star} \longrightarrow \mathrm{AC9\_star} + \mathrm{C3\_star} \tag{17}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
AC9	APAF-1-Caspase 9 complex	
C3_star	Caspase 3 cleaved	

Products

Table 23: Properties of each product.

Id	Name	SBO
AC9_star	APAF-1-Caspase 9 cleaved complex	
C3_star	Caspase 3 cleaved	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_9 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k5} \cdot [\mathrm{AC9}] \cdot [\mathrm{C3\_star}] \tag{18}$$

6.10 Reaction v8

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

Name cleaved Caspase 9 Apaf-1 binding

Reaction equation

$$\mathrm{C9\_star} + \mathrm{A} \rightleftharpoons \mathrm{AC9\_star} \tag{19}$$

Reactants

Table 24: Properties of each reactant.

Id	Name	SBO
C9_star	Caspase 9 cleaved	
A	APAF-1	

Product

Table 25: Properties of each product.

Id	Name	SBO
AC9_star	APAF-1-Caspase 9 cleaved complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_{10} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{k8} \cdot [\mathrm{C9\_star}] \cdot [\mathrm{A}] - \mathrm{k8b} \cdot [\mathrm{AC9\_star}]) \tag{20}$$

6.11 Reaction v11

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

Name cleaved Caspase 9 XIAP binding

Reaction equation

$$\mathrm{C9\_star} + \mathrm{X} \rightleftharpoons \mathrm{C9\_starX} \tag{21}$$

Reactants

Table 26: Properties of each reactant.

Id	Name	SBO
C9_star	Caspase 9 cleaved	
X	XIAP	

Product

Table 27: Properties of each product.

Id	Name	SBO
C9_starX	Caspase 9 cleaved-XIAP complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_{11} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{k11} \cdot [\mathrm{C9\_star}] \cdot [\mathrm{X}] - \mathrm{k11b} \cdot [\mathrm{C9\_starX}]) \tag{22}$$

6.12 Reaction v12

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

Name cleaved Caspase 9-Apaf-1 XIAP binding

Reaction equation

$$\mathrm{AC9\_star} + \mathrm{X} \rightleftharpoons \mathrm{AC9\_starX} \tag{23}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
AC9_star	APAF-1-Caspase 9 cleaved complex	
X	XIAP	

Product

Table 29: Properties of each product.

Id	Name	SBO
AC9_starX	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_{12} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{k12} \cdot [\mathrm{AC9\_star}] \cdot [\mathrm{X}] - \mathrm{k12b} \cdot [\mathrm{AC9\_starX}]) \tag{24}$$

6.13 Reaction v14

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

Name cleaved Caspase 9-Xiap Apaf-1 binding

Reaction equation

$$\text{C9\_starX} + \text{A} \rightleftharpoons \text{AC9\_starX} \tag{25}$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
C9_starX	Caspase 9 cleaved-XIAP complex	
A	APAF-1	

Product

Table 31: Properties of each product.

Id	Name	SBO
AC9_starX	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

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

$$v_{13} = \text{vol}\,(\text{cytosol}) \cdot (\text{k14} \cdot [\text{C9\_starX}] \cdot [\text{A}] - \text{k14b} \cdot [\text{AC9\_starX}]) \tag{26}$$

6.14 Reaction v6

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

Name Caspase 3 cleavage by cleaved Caspase 9

Reaction equation

$$\text{C3} + \text{C9\_star} \longrightarrow \text{C3\_star} + \text{C9\_star} \tag{27}$$

Reactants

Table 32: Properties of each reactant.

Id	Name	SBO
C3	Caspase 3	
C9_star	Caspase 9 cleaved	

Products

Table 33: Properties of each product.

Id	Name	SBO
C3_star	Caspase 3 cleaved	
C9_star	Caspase 9 cleaved	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_{14} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k6} \cdot [\mathrm{C3}] \cdot [\mathrm{C9\_star}] \tag{28}$$

6.15 Reaction v7

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

Name Caspase 3 cleavage by cleaved Caspase 9 - Apaf-1

Reaction equation

$$\mathrm{C3} + \mathrm{AC9\_star} \longrightarrow \mathrm{C3\_star} + \mathrm{AC9\_star} \tag{29}$$

Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
C3	Caspase 3	
AC9_star	APAF-1-Caspase 9 cleaved complex	

Products

Table 35: Properties of each product.

Id	Name	SBO
C3_star	Caspase 3 cleaved	
AC9_star	APAF-1-Caspase 9 cleaved complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_{15} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k7} \cdot [\mathrm{C3}] \cdot [\mathrm{AC9\_star}] \tag{30}$$

6.16 Reaction v16

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

Name Apaf-1 turnover

Reaction equation

$$\emptyset \longrightarrow \mathrm{A} \tag{31}$$

Product

Table 36: Properties of each product.

Id	Name	SBO
A	APAF-1	

Kinetic Law

Derived unit $\mathrm{nmol} \cdot \mathrm{s}^{-1}$

$$v_{16} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{k16prod} - \mathrm{k16} \cdot [\mathrm{A}]) \tag{32}$$

6.17 Reaction v17

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

Name Caspase 9 turnover

Reaction equation

$$\emptyset \longrightarrow \mathrm{C9} \tag{33}$$

Product

Table 37: Properties of each product.

Id	Name	SBO
C9	Caspase 9	

Kinetic Law

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

$$v_{17} = \text{vol}(\text{cytosol}) \cdot (\text{k17prod} - \text{k17} \cdot [\text{C9}]) \tag{34}$$

6.18 Reaction v18

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

Name Xiap turnover

Reaction equation

$$\emptyset \longrightarrow \text{X} \tag{35}$$

Product

Table 38: Properties of each product.

Id	Name	SBO
X	XIAP	

Kinetic Law

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

$$v_{18} = \text{vol}(\text{cytosol}) \cdot (\text{k18prod} - \text{k18} \cdot [\text{X}]) \tag{36}$$

6.19 Reaction v19

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

Name Caspase 9-Xiap degradation

Reaction equation

$$\text{C9X} \longrightarrow \emptyset \tag{37}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
C9X	Caspase 9-XIAP complex	

Kinetic Law

Derived unit $s^{-1} \cdot nmol$

$$v_{19} = \mathrm{vol}(\mathrm{cytosol}) \cdot k19 \cdot [C9X] \tag{38}$$

6.20 Reaction v20

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

Name Apaf-1-Caspase 9-Xiap degradation

Reaction equation

$$AC9X \longrightarrow \emptyset \tag{39}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
AC9X	APAF-1-Caspase 9-XIAP complex	

Kinetic Law

Derived unit $s^{-1} \cdot nmol$

$$v_{20} = \mathrm{vol}(\mathrm{cytosol}) \cdot k20 \cdot [AC9X] \tag{40}$$

6.21 Reaction v21

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

Name Apaf-1-Caspase 9 degradation

Reaction equation

$$AC9 \longrightarrow \emptyset \tag{41}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
AC9	APAF-1-Caspase 9 complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_{21} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k21} \cdot [\mathrm{AC9}] \tag{42}$$

6.22 Reaction v22

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

Name Caspase 3 turnover

Reaction equation

$$\emptyset \longrightarrow \mathrm{C3} \tag{43}$$

Product

Table 42: Properties of each product.

Id	Name	SBO
C3	Caspase 3	

Kinetic Law

Derived unit $\mathrm{nmol} \cdot \mathrm{s}^{-1}$

$$v_{22} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{k22prod} - \mathrm{k22} \cdot [\mathrm{C3}]) \tag{44}$$

6.23 Reaction v23

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

Name Caspase 3 cleaved degradation

Reaction equation

$$\mathrm{C3\_star} \longrightarrow \emptyset \tag{45}$$

Reactant

Table 43: Properties of each reactant.

Id	Name	SBO
C3_star	Caspase 3 cleaved	

Kinetic Law

Derived unit $s^{-1} \cdot nmol$

$$v_{23} = \text{vol}(\text{cytosol}) \cdot \text{k23} \cdot [\text{C3\_star}] \tag{46}$$

6.24 Reaction v24

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

Name Caspase 3 cleaved-Xiap degradation

Reaction equation

$$\text{C3\_starX} \longrightarrow \emptyset \tag{47}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
C3_starX	Caspase 3 cleaved - XIAP complex	

Kinetic Law

Derived unit $s^{-1} \cdot nmol$

$$v_{24} = \text{vol}(\text{cytosol}) \cdot \text{k24} \cdot [\text{C3\_starX}] \tag{48}$$

6.25 Reaction v25

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

Name Caspase 9 cleaved-Xiap degradation

Reaction equation

$$\text{C9\_starX} \longrightarrow \emptyset \tag{49}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
C9_starX	Caspase 9 cleaved-XIAP complex	

Kinetic Law

Derived unit $s^{-1} \cdot nmol$

$$v_{25} = \text{vol}(\text{cytosol}) \cdot \text{k25} \cdot [\text{C9\_starX}] \tag{50}$$

6.26 Reaction v26

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

Name Caspase 9 cleaved degradation

Reaction equation

$$\text{C9\_star} \longrightarrow \emptyset \tag{51}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
C9_star	Caspase 9 cleaved	

Kinetic Law

Derived unit $s^{-1} \cdot nmol$

$$v_{26} = \text{vol}(\text{cytosol}) \cdot \text{k26} \cdot [\text{C9\_star}] \tag{52}$$

6.27 Reaction v27

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

Name Apaf-1 Caspase 9 cleaved degradation

Reaction equation

$$\text{AC9\_star} \longrightarrow \emptyset \tag{53}$$

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
AC9_star	APAF-1-Caspase 9 cleaved complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_{27} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k27} \cdot [\mathrm{AC9\_star}] \tag{54}$$

6.28 Reaction v28

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

Name Apaf-1 Caspase 9 cleaved-Xiap degradation

Reaction equation

$$\mathrm{AC9\_starX} \longrightarrow \emptyset \tag{55}$$

Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
AC9_starX	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{nmol}$

$$v_{28} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k28} \cdot [\mathrm{AC9\_starX}] \tag{56}$$

7 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.

7.1 Species A

Name APAF-1

Initial concentration $20\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in v1, v13, v8, v14 and as a product in v16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} = v_{16} - v_1 - v_6 - v_{10} - v_{13} \tag{57}$$

7.2 Species C9

Name Caspase 9

Initial concentration $20\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in v1, v2, v9, v4 and as a product in v2, v17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C9} = v_2 + v_{17} - v_1 - v_2 - v_4 - v_8 \tag{58}$$

7.3 Species C9X

Name Caspase 9-XIAP complex

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

This species takes part in three reactions (as a reactant in v13, v19 and as a product in v9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C9X} = v_4 - v_6 - v_{19} \tag{59}$$

7.4 Species X

Name XIAP

Initial concentration $40\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in v9, v10, v15, v11, v12 and as a product in v18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = v_{18} - v_4 - v_5 - v_7 - v_{11} - v_{12} \tag{60}$$

7.5 Species AC9X

Name APAF-1-Caspase 9-XIAP complex

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

This species takes part in three reactions (as a reactant in v20 and as a product in v10, v13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AC9X} = v_5 + v_6 - v_{20} \tag{61}$$

7.6 Species AC9

Name APAF-1-Caspase 9 complex

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

This species takes part in six reactions (as a reactant in v3, v10, v5, v21 and as a product in v1, v3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AC9} = v_1 + v_3 - v_3 - v_5 - v_9 - v_{21} \tag{62}$$

7.7 Species C3

Name Caspase 3

Initial concentration $200\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in v2, v3, v6, v7 and as a product in v22).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C3} = v_{22} - v_2 - v_3 - v_{14} - v_{15} \tag{63}$$

7.8 Species C3_star

Name Caspase 3 cleaved

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

This species takes part in ten reactions (as a reactant in v15, v4, v5, v23 and as a product in v2, v3, v4, v5, v6, v7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C3\_star} = v_2 + v_3 + v_8 + v_9 + v_{14} + v_{15} - v_7 - v_8 - v_9 - v_{23} \tag{64}$$

7.9 Species C3_starX

Name Caspase 3 cleaved - XIAP complex

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

This species takes part in two reactions (as a reactant in v24 and as a product in v15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C3\_starX} = v_7 - v_{24} \tag{65}$$

7.10 Species C9_starX

Name Caspase 9 cleaved-XIAP complex

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

This species takes part in three reactions (as a reactant in v14, v25 and as a product in v11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C9\_starX} = v_{11} - v_{13} - v_{25} \tag{66}$$

7.11 Species C9_star

Name Caspase 9 cleaved

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

This species takes part in six reactions (as a reactant in v8, v11, v6, v26 and as a product in v4, v6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C9\_star} = v_8 + v_{14} - v_{10} - v_{11} - v_{14} - v_{26} \tag{67}$$

7.12 Species AC9_star

Name APAF-1-Caspase 9 cleaved complex

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

This species takes part in six reactions (as a reactant in v12, v7, v27 and as a product in v5, v8, v7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AC9\_star} = v_9 + v_{10} + v_{15} - v_{12} - v_{15} - v_{27} \tag{68}$$

7.13 Species AC9_starX

Name Apaf-1-Caspase 9 cleaved -XIAP complex

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

This species takes part in three reactions (as a reactant in v28 and as a product in v12, v14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AC9\_starX} = v_{12} + v_{13} - v_{28} \tag{69}$$

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