

SBML Model Report

Model name: “Legewie2006_apoptosis_NC”



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following four authors: Harish Dharuri¹, Stefan Legewie², Nils Bluethgen³ and Hanspeter Herzel⁴ at April 20th 2006 at 10:59 a. m. and last time modified at July fifth 2012 at 2:46 p. m. Table 1 provides 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	17
events	0	constraints	0
reactions	42	function definitions	0
global parameters	49	unit definitions	5
rules	0	initial assignments	0

Model Notes

This model represents the non-competitive binding of XIAP to Casapase-3 and Caspase-9. In other words, XIAP mediated feedback is abolished in this model. The authors state that this leads to bistable-reversible behaviour as depicted in Fig 4C. The wild-type model displays a bistable-irreversible profile. This shows that irreversibility requires XIAP mediated feedback.

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The model was tested on MathSBML. However, please note that the paper does not contain any figure that corresponds to simulation of the Non-Competitive model.

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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 $\text{nmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$

2.3 Unit `per_nM_per_sec`

Name `per_nM_per_sec`

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

2.4 Unit `nM`

Name `nM`

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

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 1

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	<input checked="" type="checkbox"/>	

3.1 Compartment `cytosol`

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

Name Cytosol

4 Species

This model contains 17 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	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
C9	Caspase 9	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
C9X	Caspase 9-XIAP complex	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
X	XIAP	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
AC9X	APAF-1-Caspase 9-XIAP complex	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
AC9	APAF-1-Caspase 9 complex	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
C3	Caspase 3	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
C3_star	Caspase 3 cleaved	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
C3_starX	Caspase 3 cleaved - XIAP complex	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
C9_starX	Caspase 9 cleaved-XIAP complex	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
C9_star	Caspase 9 cleaved	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
AC9_star	APAF-1-Caspase 9 cleaved complex	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
AC9_starX	Apaf-1-Caspase 9 cleaved -XIAP complex	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
C9X_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
AC9X_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
C9_starX_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
AC9_starX_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	cytosol	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square

5 Parameters

This model contains 49 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.002		<input checked="" type="checkbox"/>
kb1			0.100		<input checked="" type="checkbox"/>
k2			$5 \cdot 10^{-6}$		<input checked="" type="checkbox"/>
k3			$3.5 \cdot 10^{-4}$		<input checked="" type="checkbox"/>
k9			0.001		<input checked="" type="checkbox"/>
k9b			0.001		<input checked="" type="checkbox"/>
k10			0.001		<input checked="" type="checkbox"/>
k10b			0.001		<input checked="" type="checkbox"/>
k13			0.002		<input checked="" type="checkbox"/>
k13b			0.100		<input checked="" type="checkbox"/>
k15			0.003		<input checked="" type="checkbox"/>
k15b			0.001		<input checked="" type="checkbox"/>
k4			$2 \cdot 10^{-4}$		<input checked="" type="checkbox"/>
k5			$2 \cdot 10^{-4}$		<input checked="" type="checkbox"/>
k8			0.002		<input checked="" type="checkbox"/>
k8b			0.100		<input checked="" type="checkbox"/>
k11			0.001		<input checked="" type="checkbox"/>
k11b			0.001		<input checked="" type="checkbox"/>
k12			0.001		<input checked="" type="checkbox"/>
k12b			0.001		<input checked="" type="checkbox"/>
k14			0.002		<input checked="" type="checkbox"/>
k14b			0.100		<input checked="" type="checkbox"/>
k6			$5 \cdot 10^{-5}$		<input checked="" type="checkbox"/>
k7			0.004		<input checked="" type="checkbox"/>
k16			0.001		<input checked="" type="checkbox"/>
k16prod			0.020		<input checked="" type="checkbox"/>
k17			0.001		<input checked="" type="checkbox"/>
k17prod			0.020		<input checked="" type="checkbox"/>
k18			0.001		<input checked="" type="checkbox"/>
k18prod			0.040		<input checked="" type="checkbox"/>
k19			0.001		<input checked="" type="checkbox"/>
k20			0.001		<input checked="" type="checkbox"/>
k21			0.001		<input checked="" type="checkbox"/>
k22			0.001		<input checked="" type="checkbox"/>
k22prod			0.200		<input checked="" type="checkbox"/>
k23			0.001		<input checked="" type="checkbox"/>
k24			0.001		<input checked="" type="checkbox"/>

Id	Name	SBO	Value	Unit	Constant
k25			0.001		<input checked="" type="checkbox"/>
k26			0.001		<input checked="" type="checkbox"/>
k27			0.001		<input checked="" type="checkbox"/>
k28			0.001		<input checked="" type="checkbox"/>
k29			0.001		<input checked="" type="checkbox"/>
k30			0.001		<input checked="" type="checkbox"/>
k31			0.001		<input checked="" type="checkbox"/>
k32			0.001		<input checked="" type="checkbox"/>
a			1.000		<input checked="" type="checkbox"/>
d			1.000		<input checked="" type="checkbox"/>
k41			1.000		<input checked="" type="checkbox"/>
k42			1.000		<input checked="" type="checkbox"/>

6 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

Nº	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	$AC9 \longrightarrow \emptyset$	

Nº	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	$AC9_starX \longrightarrow \emptyset$	
29	v29	Caspase9-Xiap-Caspase3_star degradation	$C9X_C3_star \longrightarrow \emptyset$	
30	v30	Apaf-1-Caspase9-Xiap-Caspase3_star degradation	$AC9_starX_C3_star \longrightarrow \emptyset$	
31	v31	Caspase9_star-Xiap-Caspase3_star degradation	$C9_starX_C3_star \longrightarrow \emptyset$	
32	v32	Apaf-1-Caspase9_star-Xiap-Caspase3_star degradation	$AC9_starX_C3_star \longrightarrow \emptyset$	
33	v33	Cleaved-Caspase 3 binding with Xiap-Caspase 9	$C3_star + C9X \rightleftharpoons C9X_C3_star$	
34	v34	Cleaved-Caspase 3 binding with Apaf-Xiap-Caspase 9	$C3_star + AC9X \rightleftharpoons AC9X_C3_star$	
35	v35	Cleaved-Caspase 3 binding with Cleaved-Xiap-Caspase 9	$C3_star + C9_starX \rightleftharpoons C9_starX_C3_star$	
36	v36	Apaf-Xiap-cleaved Caspase 9 binding with cleaved Caspase 3	$C3_star + AC9_starX \rightleftharpoons AC9_starX_C3_star$	
37	v37	Binding of Caspase 9 to cleaved Caspase 3-Xiap	$C9 + C3_starX \rightleftharpoons C9X_C3_star$	
38	v38	Binding of Apaf-Caspase 9 to cleaved Caspase 3-Xiap	$AC9 + C3_starX \rightleftharpoons AC9X_C3_star$	
39	v39	Binding of cleaved Caspase 9 to cleaved Caspase 3-Xiap	$C9_star + C3_starX \rightleftharpoons C9_starX_C3_star$	

Nº	Id	Name	Reaction Equation	SBO
40	v40	Binding of cleaved Caspase 9-Apaf-1 to cleaved Caspase 3-Xiap	$AC9_star + C3_starX \rightleftharpoons AC9_starX_C3_star$	
41	v41	Binding of Caspase 9-Xiap-cleaved Caspase 3 with Apaf	$C9X_C3_star + A \rightleftharpoons AC9X_C3_star$	
42	v42	Binding of cleaved Caspase 9-Xiap-cleaved Caspase 3 with Apaf	$C9_starX_C3_star + A \rightleftharpoons AC9_starX_C3_star$	

6.1 Reaction v1

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

Name Caspase 9 / Apaf-1 binding

Reaction equation



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 contains undeclared units

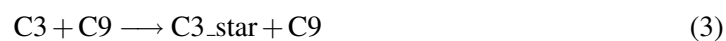
$$v_1 = \text{vol}(\text{cytosol}) \cdot (k_1 \cdot [A] \cdot [C9] - k_{b1} \cdot [AC9]) \quad (2)$$

6.2 Reaction v2

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

Name Caspase 3 cleavage by Caspase 9

Reaction equation



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 contains undeclared units

$$v_2 = \text{vol}(\text{cytosol}) \cdot k_2 \cdot [\text{C3}] \cdot [\text{C9}] \quad (4)$$

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



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 contains undeclared units

$$v_3 = \text{vol}(\text{cytosol}) \cdot k_3 \cdot [\text{C3}] \cdot [\text{AC9}] \quad (6)$$

6.4 Reaction v9

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

Name Caspase 9 Xiap binding

Reaction equation



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 contains undeclared units

$$v_4 = \text{vol}(\text{cytosol}) \cdot (k_9 \cdot [\text{C9}] \cdot [\text{X}] - k_{9b} \cdot [\text{C9X}]) \quad (8)$$

6.5 Reaction v10

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

Name Caspase 9-Apaf-1 Xiap binding

Reaction equation



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 contains undeclared units

$$v_5 = \text{vol}(\text{cytosol}) \cdot (k_{10} \cdot [\text{AC9}] \cdot [\text{X}] - k_{10b} \cdot [\text{AC9X}]) \quad (10)$$

6.6 Reaction v13

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

Name Caspase 9-Xiap Apaf-1 binding

Reaction equation



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 contains undeclared units

$$v_6 = \text{vol}(\text{cytosol}) \cdot (k_{13} \cdot [\text{C9X}] \cdot [\text{A}] - k_{13b} \cdot [\text{AC9X}]) \quad (12)$$

6.7 Reaction v15

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

Name cleaved Caspase 3-Xiap binding

Reaction equation



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 contains undeclared units

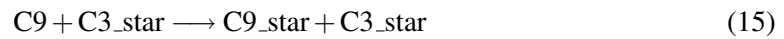
$$v_7 = \text{vol}(\text{cytosol}) \cdot (k_{15} \cdot [\text{C3_star}] \cdot [\text{X}] - k_{15b} \cdot [\text{C3_starX}]) \quad (14)$$

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



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 contains undeclared units

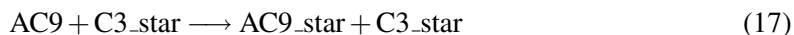
$$v_8 = \text{vol}(\text{cytosol}) \cdot k_4 \cdot [\text{C9}] \cdot [\text{C3_star}] \quad (16)$$

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



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 contains undeclared units

$$v_9 = \text{vol}(\text{cytosol}) \cdot k_5 \cdot [\text{AC9}] \cdot [\text{C3_star}] \quad (18)$$

6.10 Reaction v8

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

Name cleaved Caspase 9 Apaf-1 binding

Reaction equation



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 contains undeclared units

$$v_{10} = \text{vol}(\text{cytosol}) \cdot (k_8 \cdot [\text{C9_star}] \cdot [\text{A}] - k_{8b} \cdot [\text{AC9_star}]) \quad (20)$$

6.11 Reaction v11

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

Name cleaved Caspase 9 XIAP binding

Reaction equation



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** contains undeclared units

$$v_{11} = \text{vol}(\text{cytosol}) \cdot (k_{11} \cdot [\text{C9_star}] \cdot [\text{X}] - k_{11b} \cdot [\text{C9_starX}]) \quad (22)$$

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****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** contains undeclared units

$$v_{12} = \text{vol}(\text{cytosol}) \cdot (k_{12} \cdot [\text{AC9_star}] \cdot [\text{X}] - k_{12b} \cdot [\text{AC9_starX}]) \quad (24)$$

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



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 contains undeclared units

$$v_{13} = \text{vol}(\text{cytosol}) \cdot (k_{14} \cdot [\text{C9_starX}] \cdot [\text{A}] - k_{14b} \cdot [\text{AC9_starX}]) \quad (26)$$

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



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 contains undeclared units

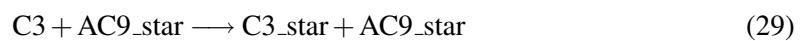
$$v_{14} = \text{vol}(\text{cytosol}) \cdot k_6 \cdot [\text{C3}] \cdot [\text{C9_star}] \quad (28)$$

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



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** contains undeclared units

$$v_{15} = \text{vol}(\text{cytosol}) \cdot k_7 \cdot [\text{C3}] \cdot [\text{AC9_star}] \quad (30)$$

6.16 Reaction v16

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

Name Apaf-1 turnover**Reaction equation****Product**

Table 36: Properties of each product.

Id	Name	SBO
A	APAF-1	

Kinetic Law**Derived unit** contains undeclared units

$$v_{16} = \text{vol}(\text{cytosol}) \cdot (k_{16\text{prod}} - k_{16} \cdot [\text{A}]) \quad (32)$$

6.17 Reaction v17

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

Name Caspase 9 turnover**Reaction equation**

Product

Table 37: Properties of each product.

Id	Name	SBO
C9	Caspase 9	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{vol}(\text{cytosol}) \cdot (k_{17\text{prod}} - k_{17} \cdot [\text{C9}]) \quad (34)$$

6.18 Reaction v18

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

Name Xiap turnover

Reaction equation



Product

Table 38: Properties of each product.

Id	Name	SBO
X	XIAP	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol}(\text{cytosol}) \cdot (k_{18\text{prod}} - k_{18} \cdot [\text{X}]) \quad (36)$$

6.19 Reaction v19

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

Name Caspase 9-Xiap degradation

Reaction equation



Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
C9X	Caspase 9-XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{vol}(\text{cytosol}) \cdot k_{19} \cdot [\text{C9X}] \quad (38)$$

6.20 Reaction v20

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

Name Apaf-1-Caspase 9-Xiap degradation

Reaction equation



Reactant

Table 40: Properties of each reactant.

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

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}(\text{cytosol}) \cdot k_{20} \cdot [\text{AC9X}] \quad (40)$$

6.21 Reaction v21

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

Name Apaf-1-Caspase 9 degradation

Reaction equation



Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
AC9	APAF-1-Caspase 9 complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{vol}(\text{cytosol}) \cdot k_{21} \cdot [\text{AC9}] \quad (42)$$

6.22 Reaction v22

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

Name Caspase 3 turnover

Reaction equation



Product

Table 42: Properties of each product.

Id	Name	SBO
C3	Caspase 3	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{vol}(\text{cytosol}) \cdot (k_{22\text{prod}} - k_{22} \cdot [\text{C3}]) \quad (44)$$

6.23 Reaction v23

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

Name Caspase 3 cleaved degradation

Reaction equation



Reactant

Table 43: Properties of each reactant.

Id	Name	SBO
C3_star	Caspase 3 cleaved	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{vol}(\text{cytosol}) \cdot k_{23} \cdot [\text{C3_star}] \quad (46)$$

6.24 Reaction v24

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

Name Caspase 3 cleaved-Xiap degradation

Reaction equation



Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
C3_starX	Caspase 3 cleaved - XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \text{vol}(\text{cytosol}) \cdot k_{24} \cdot [\text{C3_starX}] \quad (48)$$

6.25 Reaction v25

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

Name Caspase 9 cleaved-Xiap degradation

Reaction equation



Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
C9_starX	Caspase 9 cleaved-XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \text{vol}(\text{cytosol}) \cdot k_{25} \cdot [\text{C9_starX}] \quad (50)$$

6.26 Reaction v26

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

Name Caspase 9 cleaved degradation

Reaction equation



Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
C9_star	Caspase 9 cleaved	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \text{vol}(\text{cytosol}) \cdot k_{26} \cdot [\text{C9_star}] \quad (52)$$

6.27 Reaction v27

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

Name Apaf-1 Caspase 9 cleaved degradation

Reaction equation



Reactant

Table 47: Properties of each reactant.

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

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \text{vol}(\text{cytosol}) \cdot k_{27} \cdot [\text{AC9_star}] \quad (54)$$

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



Reactant

Table 48: Properties of each reactant.

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

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \text{vol}(\text{cytosol}) \cdot k_{28} \cdot [\text{AC9_starX}] \quad (56)$$

6.29 Reaction v29

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

Name Caspase9-Xiap-Caspase3_star degradation

Reaction equation



Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
C9X_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \text{vol}(\text{cytosol}) \cdot k_{29} \cdot [\text{C9X_C3_star}] \quad (58)$$

6.30 Reaction v30

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

Name Apaf-1-Caspase9-Xiap-Caspase3_star degradation

Reaction equation



Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
AC9_starX_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \text{vol}(\text{cytosol}) \cdot k_{30} \cdot [\text{AC9_starX_C3_star}] \quad (60)$$

6.31 Reaction v31

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

Name Caspase9_star-Xiap-Caspase3_star degradation

Reaction equation



Reactant

Table 51: Properties of each reactant.

Id	Name	SBO
C9_starX_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \text{vol}(\text{cytosol}) \cdot k_{31} \cdot [\text{C9_starX_C3_star}] \quad (62)$$

6.32 Reaction v32

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

Name Apaf-1-Caspase9_star-Xiap-Caspase3_star degradation

Reaction equation



Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
AC9_starX_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \text{vol}(\text{cytosol}) \cdot k_{32} \cdot [\text{AC9_starX_C3_star}] \quad (64)$$

6.33 Reaction v33

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

Name Cleaved-Caspase 3 binding with Xiap-Caspase 9

Reaction equation



Reactants

Table 53: Properties of each reactant.

Id	Name	SBO
C3_star	Caspase 3 cleaved	
C9X	Caspase 9-XIAP complex	

Product

Table 54: Properties of each product.

Id	Name	SBO
C9X_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

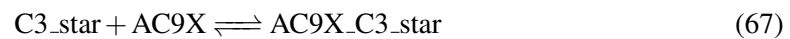
$$v_{33} = \text{vol}(\text{cytosol}) \cdot (a \cdot k_{15} \cdot [\text{C3_star}] \cdot [\text{C9X}] - d \cdot k_{15b} \cdot [\text{C9X_C3_star}]) \quad (66)$$

6.34 Reaction v34

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

Name Cleaved-Caspase 3 binding with Apaf-Xiap-Caspase 9

Reaction equation



Reactants

Table 55: Properties of each reactant.

Id	Name	SBO
C3_star	Caspase 3 cleaved	
AC9X	APAF-1-Caspase 9-XIAP complex	

Product

Table 56: Properties of each product.

Id	Name	SBO
AC9X_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \text{vol}(\text{cytosol}) \cdot (a \cdot k_{15} \cdot [\text{C3_star}] \cdot [\text{AC9X}] - d \cdot k_{15b} \cdot [\text{AC9X_C3_star}]) \quad (68)$$

6.35 Reaction v35

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

Name Cleaved-Caspase 3 binding with Cleaved-Xiap-Caspase 9

Reaction equation



Reactants

Table 57: Properties of each reactant.

Id	Name	SBO
C3_star	Caspase 3 cleaved	
C9_starX	Caspase 9 cleaved-XIAP complex	

Product

Table 58: Properties of each product.

Id	Name	SBO
C9_starX_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \text{vol}(\text{cytosol}) \cdot (a \cdot k_{15} \cdot [\text{C3_star}] \cdot [\text{C9_starX}] - d \cdot k_{15b} \cdot [\text{C9_starX_C3_star}]) \quad (70)$$

6.36 Reaction v36

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

Name Apaf-Xiap-cleaved Caspase 9 binding with cleaved Caspase 3

Reaction equation



Reactants

Table 59: Properties of each reactant.

Id	Name	SBO
C3_star	Caspase 3 cleaved	
AC9_starX	Apaf-1-Caspase 9 cleaved -XIAP complex	

Product

Table 60: Properties of each product.

Id	Name	SBO
AC9_starX_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \text{vol}(\text{cytosol}) \cdot (a \cdot k_{15} \cdot [C3_star] \cdot [AC9_starX] - d \cdot k_{15b} \cdot [AC9_starX_C3_star]) \quad (72)$$

6.37 Reaction v37

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

Name Binding of Caspase 9 to cleaved Caspase 3-Xiap

Reaction equation



Reactants

Table 61: Properties of each reactant.

Id	Name	SBO
C9	Caspase 9	
C3_starX	Caspase 3 cleaved - XIAP complex	

Product

Table 62: Properties of each product.

Id	Name	SBO
C9X_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

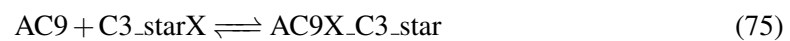
$$v_{37} = \text{vol}(\text{cytosol}) \cdot (a \cdot k_9 \cdot [\text{C9}] \cdot [\text{C3_starX}] - d \cdot k_{9b} \cdot [\text{C9X_C3_star}]) \quad (74)$$

6.38 Reaction v38

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

Name Binding of Apaf-Caspase 9 to cleaved Caspase 3-Xiap

Reaction equation



Reactants

Table 63: Properties of each reactant.

Id	Name	SBO
AC9	APAF-1-Caspase 9 complex	
C3_starX	Caspase 3 cleaved - XIAP complex	

Product

Table 64: Properties of each product.

Id	Name	SBO
AC9X_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \text{vol}(\text{cytosol}) \cdot (a \cdot k_9 \cdot [\text{AC9}] \cdot [\text{C3_starX}] - d \cdot k_{9b} \cdot [\text{AC9X_C3_star}]) \quad (76)$$

6.39 Reaction v39

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

Name Binding of cleaved Caspase 9 to cleaved Caspase 3-Xiap

Reaction equation



Reactants

Table 65: Properties of each reactant.

Id	Name	SBO
C9_star	Caspase 9 cleaved	
C3_starX	Caspase 3 cleaved - XIAP complex	

Product

Table 66: Properties of each product.

Id	Name	SBO
C9_starX_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = \text{vol}(\text{cytosol}) \cdot (a \cdot k_9 \cdot [\text{C9_star}] \cdot [\text{C3_starX}] - d \cdot k_{9b} \cdot [\text{C9_starX_C3_star}]) \quad (78)$$

6.40 Reaction v40

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

Name Binding of cleaved Caspase 9-Apaf-1 to cleaved Caspase 3-Xiap

Reaction equation



Reactants

Table 67: Properties of each reactant.

Id	Name	SBO
AC9_star	APAF-1-Caspase 9 cleaved complex	
C3_starX	Caspase 3 cleaved - XIAP complex	

Product

Table 68: Properties of each product.

Id	Name	SBO
AC9_starX_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

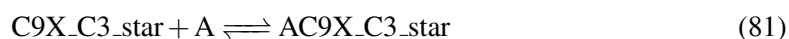
$$v_{40} = \text{vol}(\text{cytosol}) \cdot (a \cdot k_9 \cdot [\text{AC9_star}] \cdot [\text{C3_starX}] - d \cdot k_{9b} \cdot [\text{AC9_starX_C3_star}]) \quad (80)$$

6.41 Reaction v41

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

Name Binding of Caspase 9-Xiap-cleaved Caspase 3 with Apaf

Reaction equation



Reactants

Table 69: Properties of each reactant.

Id	Name	SBO
C9X_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	
A	APAF-1	

Product

Table 70: Properties of each product.

Id	Name	SBO
AC9X_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = \text{vol}(\text{cytosol}) \cdot (a \cdot k_1 \cdot [\text{C9X_C3_star}] \cdot [\text{A}] - d \cdot k_{b1} \cdot [\text{AC9X_C3_star}]) \quad (82)$$

6.42 Reaction v42

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

Name Binding of cleaved Caspase 9-Xiap-cleaved Caspase 3 with Apaf

Reaction equation



Reactants

Table 71: Properties of each reactant.

Id	Name	SBO
C9_starX_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	
A	APAF-1	

Product

Table 72: Properties of each product.

Id	Name	SBO
AC9_starX_C3_star	Apaf-1-Caspase 9 cleaved -XIAP complex	

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = \text{vol}(\text{cytosol}) \cdot (a \cdot k1 \cdot [\text{C9_starX_C3_star}] \cdot [\text{A}] - d \cdot kb1 \cdot [\text{AC9_starX_C3_star}]) \quad (84)$$

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.

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.

7.1 Species A

Name APAF-1

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

This species takes part in seven reactions (as a reactant in [v1](#), [v13](#), [v8](#), [v14](#), [v41](#), [v42](#) and as a product in [v16](#)).

$$\frac{d}{dt}A = v_{16} - v_1 - v_6 - v_{10} - v_{13} - v_{41} - v_{42} \quad (85)$$

7.2 Species C9

Name Caspase 9

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

This species takes part in seven reactions (as a reactant in [v1](#), [v2](#), [v9](#), [v4](#), [v37](#) and as a product in [v2](#), [v17](#)).

$$\frac{d}{dt}C9 = v_2 + v_{17} - v_1 - v_2 - v_4 - v_8 - v_{37} \quad (86)$$

7.3 Species C9X

Name Caspase 9-XIAP complex

Initial concentration 0 nmol · l⁻¹

This species takes part in four reactions (as a reactant in v13, v19, v33 and as a product in v9).

$$\frac{d}{dt}C9X = v_4 - v_6 - v_{19} - v_{33} \quad (87)$$

7.4 Species X

Name XIAP

Initial concentration 40 nmol · l⁻¹

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

$$\frac{d}{dt}X = v_{18} - v_4 - v_5 - v_7 - v_{11} - v_{12} \quad (88)$$

7.5 Species AC9X

Name APAF-1-Caspase 9-XIAP complex

Initial concentration 0 nmol · l⁻¹

This species takes part in four reactions (as a reactant in v20, v34 and as a product in v10, v13).

$$\frac{d}{dt}AC9X = v_5 + v_6 - v_{20} - v_{34} \quad (89)$$

7.6 Species AC9

Name APAF-1-Caspase 9 complex

Initial concentration 0 nmol · l⁻¹

This species takes part in seven reactions (as a reactant in v3, v10, v5, v21, v38 and as a product in v1, v3).

$$\frac{d}{dt}AC9 = v_1 + v_3 - v_3 - v_5 - v_9 - v_{21} - v_{38} \quad (90)$$

7.7 Species C3

Name Caspase 3

Initial concentration 200 nmol · l⁻¹

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

$$\frac{d}{dt}C3 = v_{22} - v_2 - v_3 - v_{14} - v_{15} \quad (91)$$

7.8 Species C3_star

Name Caspase 3 cleaved

Initial concentration 0 nmol · l⁻¹

This species takes part in 14 reactions (as a reactant in v15, v4, v5, v23, v33, v34, v35, v36 and as a product in v2, v3, v4, v5, v6, v7).

$$\begin{aligned} \frac{d}{dt}C3_star = & v_2 + v_3 + v_8 + v_9 + v_{14} + v_{15} - v_7 \\ & - v_8 - v_9 - v_{23} - v_{33} - v_{34} - v_{35} - v_{36} \end{aligned} \quad (92)$$

7.9 Species C3_starX

Name Caspase 3 cleaved - XIAP complex

Initial concentration 0 nmol · l⁻¹

This species takes part in six reactions (as a reactant in v24, v37, v38, v39, v40 and as a product in v15).

$$\frac{d}{dt}C3_starX = v_7 - v_{24} - v_{37} - v_{38} - v_{39} - v_{40} \quad (93)$$

7.10 Species C9_starX

Name Caspase 9 cleaved-XIAP complex

Initial concentration 0 nmol · l⁻¹

This species takes part in four reactions (as a reactant in v14, v25, v35 and as a product in v11).

$$\frac{d}{dt}C9_starX = v_{11} - v_{13} - v_{25} - v_{35} \quad (94)$$

7.11 Species C9_star

Name Caspase 9 cleaved

Initial concentration 0 nmol · l⁻¹

This species takes part in seven reactions (as a reactant in v8, v11, v6, v26, v39 and as a product in v4, v6).

$$\frac{d}{dt}C9_star = v_8 + v_{14} - v_{10} - v_{11} - v_{14} - v_{26} - v_{39} \quad (95)$$

7.12 Species AC9_star

Name APAF-1-Caspase 9 cleaved complex

Initial concentration 0 nmol · l⁻¹

This species takes part in seven reactions (as a reactant in v12, v7, v27, v40 and as a product in v5, v8, v7).

$$\frac{d}{dt}AC9_star = v_9 + v_{10} + v_{15} - v_{12} - v_{15} - v_{27} - v_{40} \quad (96)$$

7.13 Species AC9_starX

Name Apaf-1-Caspase 9 cleaved -XIAP complex

Initial concentration 0 nmol · l⁻¹

This species takes part in four reactions (as a reactant in v28, v36 and as a product in v12, v14).

$$\frac{d}{dt}AC9_starX = v_{12} + v_{13} - v_{28} - v_{36} \quad (97)$$

7.14 Species C9X_C3_star

Name Apaf-1-Caspase 9 cleaved -XIAP complex

Initial concentration 0 nmol · l⁻¹

This species takes part in four reactions (as a reactant in v29, v41 and as a product in v33, v37).

$$\frac{d}{dt}C9X_C3_star = v_{33} + v_{37} - v_{29} - v_{41} \quad (98)$$

7.15 Species AC9X_C3_star

Name Apaf-1-Caspase 9 cleaved -XIAP complex

Initial concentration 0 nmol · l⁻¹

This species takes part in three reactions (as a product in v34, v38, v41).

$$\frac{d}{dt} \text{AC9X_C3_star} = v_{34} + v_{38} + v_{41} \quad (99)$$

7.16 Species C9_starX_C3_star

Name Apaf-1-Caspase 9 cleaved -XIAP complex

Initial concentration 0 nmol · l⁻¹

This species takes part in four reactions (as a reactant in v31, v42 and as a product in v35, v39).

$$\frac{d}{dt} \text{C9_starX_C3_star} = v_{35} + v_{39} - v_{31} - v_{42} \quad (100)$$

7.17 Species AC9_starX_C3_star

Name Apaf-1-Caspase 9 cleaved -XIAP complex

Initial concentration 0 nmol · l⁻¹

This species takes part in five reactions (as a reactant in v30, v32 and as a product in v36, v40, v42).

$$\frac{d}{dt} \text{AC9_starX_C3_star} = v_{36} + v_{40} + v_{42} - v_{30} - v_{32} \quad (101)$$

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