SBML Model Report

Model name: "Rehm2006_Caspase"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Lukas Endler[1] at July 30th 2010 at 3:23 p. m. and last time modified at April eighth 2016 at 4:16 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	2
species types	0	species	27
events	1	constraints	0
reactions	56	function definitions	0
global parameters	99	unit definitions	7
rules	18	initial assignments	6

Model Notes

This is the standard model described in the article:
Systems analysis of effector caspase activation and its control by X-linked inhibitor of apoptosis protein.
Rehm M, Huber HJ, Dussmann H, Prehn JH. EMBO J. 2006 Sep 20;25(18):4338-49. Epub 2006 Aug 24. PMID:16932741, doi:10.1038/sj.emboj.7601295;
Abstract:
Activation of effector caspases is a final step during apoptosis. Single-cell imaging studies have

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demonstrated that this process may occur as a rapid, all-or-none response, triggering a complete substrate cleavage within 15 min. Based on biochemical data from HeLa cells, we have developed a computational model of apoptosome-dependent caspase activation that was sufficient to remodel the rapid kinetics of effector caspase activation observed in vivo. Sensitivity analyses predicted a critical role for caspase-3-dependent feedback signalling and the X-linked-inhibitor-of-apoptosis-protein (XIAP), but a less prominent role for the XIAP antagonist Smac. Single-cell experiments employing a caspase fluorescence resonance energy transfer substrate verified these model predictions qualitatively and quantitatively. XIAP was predicted to control this all-or-none response, with concentrations as high as 0.15 microM enabling, but concentrations >0.30 microM significantly blocking substrate cleavage. Overexpression of XIAP within these threshold concentrations produced cells showing slow effector caspase activation and submaximal substrate cleavage. Our study supports the hypothesis that high levels of XIAP control caspase activation and substrate cleavage, and may promote apoptosis resistance and sublethal caspase activation in vivo.

This model is slightly altered from the description in the article. Cytochrome C and SMAC release from the mitochondrion is modelled as simple first order kinetics, giving the same form as the (integrated) equations in the supplement of the article. The apoptosome formation is modelled equally - and independent of the Cytochrome C release. The speed is either limited by the Apaf1 or ProCaspase9 concentration, whichever is higher, symbolised via the parameter with the ID apolim.
Also, once the substrate concentration falls below 1 percent, the event Production_Breakdown is triggered, leading to a breakdown of XIAP and procaspase3 production and turning off of the enhanced/proteosomal degradation (degradation rate for reactions 38,39,40,43,44,46,48,50,51 changes from 0.0347 to 0.0058).

Originally created by libAntimony v1.3 (using libSBML 3.4.1)

2 Unit Definitions

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

2.1 Unit `time`

Name min

Definition 60 s

2.2 Unit `substance`

Name micromole

Definition $\mu\mathrm{mol}$

2.3 Unit `uM`

Name microM

Definition $\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

2.4 Unit `uM_per_min`

Name uM/min

Definition $\mu\mathrm{mol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$

2.5 Unit `per_uM_per_min`

Name 1/(uM*min)

Definition $\mu\mathrm{mol}^{-1} \cdot 1 \cdot (60\ \mathrm{s})^{-1}$

2.6 Unit `per_uM2_per_min`

Name 1/(uM$\hat{2}$*min)

Definition $\mu\mathrm{mol}^{-2} \cdot \mathrm{l}^{2} \cdot (60\ \mathrm{s})^{-1}$

2.7 Unit `per_min`

Name 1/min

Definition $(60\ \mathrm{s})^{-1}$

2.8 Unit `volume`

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

Definition l

2.9 Unit `area`

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

Definition m^2

2.10 Unit `length`

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

Definition m

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`cell`		0000290	3	1	litre	☑	
`mito`	mitochondrium	0000290	3	1	litre	☑	

3.1 Compartment `cell`

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

SBO:0000290 physical compartment

3.2 Compartment `mito`

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

Name mitochondrium

SBO:0000290 physical compartment

4 Species

This model contains 27 species. Section 10 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
PC3	ProCasp3	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
XIAP		cell	$\mu mol \cdot l^{-1}$	⊟	⊟
C9	Casp9(p35-p12)	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
PC9	ProCasp9	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
C3		cell	$\mu mol \cdot l^{-1}$	⊟	⊟
C9P	Casp9(p35-p10)	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
XIAP_C3	XIAP-Casp3	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
XIAP_C9	XIAP-Casp9	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
XIAP_C9_C3	XIAP-Casp9-Casp3	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
XIAP_p2frag	XIAP-p2 fragment	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
XIAP_p2frag_C3	XIAP-p2frag-Casp3	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
BIR12		cell	$\mu mol \cdot l^{-1}$	⊟	⊟
BIR12_C3	BIR12-Casp3	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
BIR3R		cell	$\mu mol \cdot l^{-1}$	⊟	⊟
BIR3R_C9	BIR3R-Casp9	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
BIR3R_p2frag	BIR3R-p2frag	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
XIAP_2SMAC	XIAP-2*SMAC	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
BIR12_SMAC	BIR12-SMAC	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
BIR3R_SMAC	BIR3R-SMAC	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
SMAC		cell	$\mu mol \cdot l^{-1}$	⊟	⊟
APAF1		cell	$\mu mol \cdot l^{-1}$	⊟	⊟
XIAP_p2frag_2SMAC	XIAP-p2frag-2*SMAC	cell	$\mu mol \cdot l^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
Substrate	Casp3 Substrate	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
ClvgPrds	Clevage Products	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
SMAC_mito	SMAC in mitochondrium	mito	$\mu mol \cdot l^{-1}$	⊟	⊟
CytC_mit	Cytochrome C in mitochondrium	mito	$\mu mol \cdot l^{-1}$	⊟	⊟
CytC_cell	cytosolic Cytochrome C	cell	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 99 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$4.68 \cdot 10^{-4}$	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	⊟
k1r			0.004	$(60\ s)^{-1}$	⊟
k2			$7.308 \cdot 10^{-4}$	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	⊟
k2r			0.012	$(60\ s)^{-1}$	⊟
k3			6.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k4			12.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k5			48.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k6			2.400	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k7			156.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k7r			0.144	$(60\ s)^{-1}$	☑
k8			156.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k8r			0.144	$(60\ s)^{-1}$	☑
k9			156.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k9r			0.144	$(60\ s)^{-1}$	☑
k10			156.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k10r			0.144	$(60\ s)^{-1}$	☑
k11			12.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k12			12.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k13			12.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k14			12.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k15			12.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k16			12.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k17			12.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k18			12.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k19			12.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k20			12.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k21			156.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k21r			0.144	$(60\ s)^{-1}$	☑
k22			156.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k22r			0.144	$(60\ s)^{-1}$	☑
k23			156.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k23r			0.144	$(60\ s)^{-1}$	☑
k24			0.000		☑
k25			0.000		☑

Id	Name	SBO	Value	Unit	Constant
k26			420.000	$\mu mol^{-2} \cdot l^2 \cdot (60\ s)^{-1}$	☑
k26r			0.133	$(60\ s)^{-1}$	☑
k27			420.000	$\mu mol^{-2} \cdot l^2 \cdot (60\ s)^{-1}$	☑
k27r			156.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k28			420.000	$\mu mol^{-2} \cdot l^2 \cdot (60\ s)^{-1}$	☑
k28r			156.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k29			420.000	$\mu mol^{-2} \cdot l^2 \cdot (60\ s)^{-1}$	☑
k29r			156.000	$\mu mol^{-2} \cdot l^2 \cdot (60\ s)^{-1}$	☑
k30			4.450	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k30r			31.900	$(60\ s)^{-1}$	☑
k31			0.330	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k31r			14.200	$(60\ s)^{-1}$	☑
k32			4.450	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k32r			156.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k33			0.330	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k33r			156.000	$\mu mol^{-1} \cdot 1 \cdot (60\ s)^{-1}$	☑
k34			420.000	$\mu mol^{-2} \cdot l^2 \cdot (60\ s)^{-1}$	☑
k34r			156.000	$(60\ s)^{-1}$	☑
k35			0.006	$(60\ s)^{-1}$	☑
k36			0.006	$(60\ s)^{-1}$	☑
k37			0.006	$(60\ s)^{-1}$	☑
k38			0.035	$(60\ s)^{-1}$	⊟
k39			0.035	$(60\ s)^{-1}$	⊟
k40			0.035	$(60\ s)^{-1}$	⊟
k41			0.006	$(60\ s)^{-1}$	☑
k42			0.035	$(60\ s)^{-1}$	☑
k43			0.035	$(60\ s)^{-1}$	⊟
k44			0.035	$(60\ s)^{-1}$	⊟
k45			0.006	$(60\ s)^{-1}$	☑
k46			0.035	$(60\ s)^{-1}$	⊟
k47			0.006	$(60\ s)^{-1}$	☑
k48			0.035	$(60\ s)^{-1}$	⊟
k49			0.006	$(60\ s)^{-1}$	☑
k50			0.006	$(60\ s)^{-1}$	⊟

Id	Name	SBO	Value	Unit	Constant
k51			0.035	$(60\ \mathrm{s})^{-1}$	⊟
k52			0.006	$(60\ \mathrm{s})^{-1}$	☑
k53			12.000	$\mu\mathrm{mol}^{-1} \cdot 1 \cdot (60\ \mathrm{s})^{-1}$	☑
th_SMAC	t_SMAC_0.5		7.000	60 s	☑
apo_lim	limiting factor for apoptosome formation		0.000	$\mu\mathrm{mol} \cdot 1^{-1}$	⊟
th_Apop	t_Apop_0.5		2.300	60 s	☑
th_CytC			1.500	60 s	☑
SMAC_norm	free SMAC per XIAP		0.000	dimensionless	⊟
XIAP_ini	initial XIAP conc		0.000	$\mu\mathrm{mol} \cdot 1^{-1}$	⊟
XIAP_2SMAC_norm	XIAP2*SMAC per XIAP		0.000	dimensionless	⊟
C9norm	normalised Casp-9		0.000	dimensionless	⊟
C9_tot	Caspase9 tot		0.000	$\mu\mathrm{mol} \cdot 1^{-1}$	⊟
C9Pnorm	normalised Casp9-P		0.000	dimensionless	⊟
C3norm	normalised Casp-3		0.000	dimensionless	⊟
C3_tot	Caspase3 tot		0.000	$\mu\mathrm{mol} \cdot 1^{-1}$	⊟
PC3norm	normalised Procasp-3		0.000	dimensionless	⊟
SMAC_rel	percent SMAC release		0.000	dimensionless	⊟
SMAC_tot	total SMAC		0.000	$\mu\mathrm{mol} \cdot 1^{-1}$	⊟
Apoform	percent Apoptosome formation		0.000	dimensionless	⊟
XIAP_norm			0.000	dimensionless	⊟
XIAP_C3_norm			0.000	dimensionless	⊟
XIAP_C9_norm			0.000	dimensionless	⊟
XIAP_p2frag_norm			0.000	dimensionless	⊟
BIR12_norm			0.000	dimensionless	⊟
BIR3R_norm			0.000	dimensionless	⊟
BIR12_C3_norm			0.000	dimensionless	⊟
BIR3R_C9_norm			0.000	dimensionless	⊟
BIR3R_p2frag_norm			0.000	dimensionless	⊟
S_breakdown			0.010	$\mu\mathrm{mol} \cdot 1^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
CytC_tot			0.000	$\mu mol \cdot l^{-1}$	⊟
APAF1_tot			0.000	$\mu mol \cdot l^{-1}$	⊟

6 Initialassignments

This is an overview of six initialassignments.

6.1 Initialassignment XIAP_ini

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

Math [XIAP]

6.2 Initialassignment C9_tot

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

Math [PC9]

6.3 Initialassignment C3_tot

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

Math [PC3]

6.4 Initialassignment SMAC_tot

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

Math [SMAC_mito]

6.5 Initialassignment CytC_tot

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

Math [CytC_mit]

6.6 Initialassignment APAF1_tot

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

Math [APAF1]

7 Rules

This is an overview of 18 rules.

7.1 Rule apo_lim

Rule apo_lim is an assignment rule for parameter apo_lim:

$$\text{apo\_lim} = \begin{cases} [\text{PC9}] & \text{if } [\text{PC9}] < [\text{APAF1}] \\ [\text{APAF1}] & \text{otherwise} \end{cases} \tag{1}$$

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

7.2 Rule SMAC_norm

Rule SMAC_norm is an assignment rule for parameter SMAC_norm:

$$\text{SMAC\_norm} = \frac{[\text{SMAC}]}{\text{XIAP\_ini}} \tag{2}$$

Derived unit dimensionless

7.3 Rule XIAP_2SMAC_norm

Rule XIAP_2SMAC_norm is an assignment rule for parameter XIAP_2SMAC_norm:

$$\text{XIAP\_2SMAC\_norm} = \frac{[\text{XIAP\_2SMAC}]}{\text{XIAP\_ini}} \tag{3}$$

Derived unit dimensionless

7.4 Rule C9norm

Rule C9norm is an assignment rule for parameter C9norm:

$$\text{C9norm} = \frac{[\text{C9}]}{\text{C9\_tot}} \tag{4}$$

Derived unit dimensionless

7.5 Rule C9Pnorm

Rule C9Pnorm is an assignment rule for parameter C9Pnorm:

$$\text{C9Pnorm} = \frac{[\text{C9P}]}{\text{C9\_tot}} \tag{5}$$

Derived unit dimensionless

7.6 Rule C3norm

Rule C3norm is an assignment rule for parameter C3norm:

$$\text{C3norm} = \frac{[\text{C3}]}{\text{C3\_tot}} \tag{6}$$

Derived unit dimensionless

7.7 Rule PC3norm

Rule PC3norm is an assignment rule for parameter PC3norm:

$$\text{PC3norm} = \frac{[\text{PC3}]}{\text{C3\_tot}} \tag{7}$$

Derived unit dimensionless

7.8 Rule SMAC_rel

Rule SMAC_rel is an assignment rule for parameter SMAC_rel:

$$\text{SMAC\_rel} = 1 - \frac{[\text{SMAC\_mito}]}{\text{SMAC\_tot}} \tag{8}$$

7.9 Rule Apoform

Rule Apoform is an assignment rule for parameter Apoform:

$$\text{Apoform} = 1 - \frac{[\text{PC9}]}{\text{C9\_tot}} \tag{9}$$

7.10 Rule XIAP_norm

Rule XIAP_norm is an assignment rule for parameter XIAP_norm:

$$\text{XIAP\_norm} = \frac{[\text{XIAP}]}{\text{XIAP\_ini}} \tag{10}$$

Derived unit dimensionless

7.11 Rule XIAP_C3_norm

Rule XIAP_C3_norm is an assignment rule for parameter XIAP_C3_norm:

$$\text{XIAP\_C3\_norm} = \frac{[\text{XIAP\_C3}] + [\text{XIAP\_C9\_C3}]}{\text{XIAP\_ini}} \tag{11}$$

Derived unit dimensionless

7.12 Rule XIAP_C9_norm

Rule XIAP_C9_norm is an assignment rule for parameter XIAP_C9_norm:

$$\text{XIAP\_C9\_norm} = \frac{[\text{XIAP\_C9}] + [\text{XIAP\_C9\_C3}]}{\text{XIAP\_ini}} \tag{12}$$

Derived unit dimensionless

7.13 Rule XIAP_p2frag_norm

Rule XIAP_p2frag_norm is an assignment rule for parameter XIAP_p2frag_norm:

$$\text{XIAP\_p2frag\_norm} = \frac{[\text{XIAP\_p2frag}] + [\text{XIAP\_p2frag\_C3}]}{\text{XIAP\_ini}} \tag{13}$$

Derived unit dimensionless

7.14 Rule BIR12_norm

Rule BIR12_norm is an assignment rule for parameter BIR12_norm:

$$\text{BIR12\_norm} = \frac{[\text{BIR12}]}{\text{XIAP\_ini}} \tag{14}$$

Derived unit dimensionless

7.15 Rule BIR3R_norm

Rule BIR3R_norm is an assignment rule for parameter BIR3R_norm:

$$\text{BIR3R\_norm} = \frac{[\text{BIR3R}]}{\text{XIAP\_ini}} \tag{15}$$

Derived unit dimensionless

7.16 Rule BIR12_C3_norm

Rule BIR12_C3_norm is an assignment rule for parameter BIR12_C3_norm:

$$\text{BIR12\_C3\_norm} = \frac{[\text{BIR12\_C3}]}{\text{XIAP\_ini}} \tag{16}$$

Derived unit dimensionless

7.17 Rule BIR3R_C9_norm

Rule BIR3R_C9_norm is an assignment rule for parameter BIR3R_C9_norm:

$$\text{BIR3R\_C9\_norm} = \frac{[\text{BIR3R\_C9}]}{\text{XIAP\_ini}} \tag{17}$$

Derived unit dimensionless

7.18 Rule BIR3R_p2frag_norm

Rule BIR3R_p2frag_norm is an assignment rule for parameter BIR3R_p2frag_norm:

$$\text{BIR3R\_p2frag\_norm} = \frac{[\text{BIR3R\_p2frag}]}{\text{XIAP\_ini}} \tag{18}$$

Derived unit dimensionless

8 Event

This is an overview of one event. Each event is initiated whenever its trigger condition switches from false to true. A delay function postpones the effects of an event to a later time point. At the time of execution, an event can assign values to species, parameters or compartments if these are not set to constant.

8.1 Event Production_Breakdown

Trigger condition

$$[\text{Substrate}] < \text{S\_breakdown} \tag{19}$$

Assignments

$$\text{k51} = 0.0058 \tag{20}$$
$$\text{k50} = 0.0058 \tag{21}$$
$$\text{k48} = 0.0058 \tag{22}$$
$$\text{k46} = 0.0058 \tag{23}$$
$$\text{k44} = 0.0058 \tag{24}$$
$$\text{k43} = 0.0058 \tag{25}$$
$$\text{k40} = 0.0058 \tag{26}$$
$$\text{k39} = 0.0058 \tag{27}$$
$$\text{k38} = 0.0058 \tag{28}$$
$$\text{k2r} = 0 \tag{29}$$
$$\text{k2} = 0 \tag{30}$$
$$\text{k1r} = 0 \tag{31}$$
$$\text{k1} = 0 \tag{32}$$

9 Reactions

This model contains 56 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	reaction1	ProCaspase3 Production	$\emptyset \rightleftharpoons PC3$	0000393
2	reaction2	XIAP Production	$\emptyset \rightleftharpoons XIAP$	0000393
3	reaction3		$C9 + PC3 \rightleftharpoons C3 + C9$	0000297
4	reaction4		$C9 + C3 \rightleftharpoons C9P + C3$	0000231
5	reaction5		$C9P + PC3 \rightleftharpoons C9P + C3$	0000231
6	reaction6		$PC3 + C3 \rightleftharpoons 2\,C3$	0000344
7	reaction7		$C3 + XIAP \rightleftharpoons XIAP\_C3$	0000526
8	reaction8		$C3 + XIAP\_C9 \rightleftharpoons XIAP\_C9\_C3$	0000526
9	reaction9		$C3 + XIAP\_p2frag \rightleftharpoons XIAP\_p2frag\_C3$	0000526
10	reaction10		$C3 + BIR12 \rightleftharpoons BIR12\_C3$	0000526
11	reaction11		$C3 + XIAP \rightleftharpoons BIR12 + BIR3R + C3$	0000526
12	reaction12		$C3 + XIAP\_C9 \rightleftharpoons BIR12 + BIR3R\_C9 + C3$	0000344
13	reaction13		$C3 + XIAP\_C3 \rightleftharpoons C3 + BIR12\_C3 + BIR3R$	0000344
14	reaction14		$C3 + XIAP\_p2frag \rightleftharpoons C3 + BIR12 + BIR3R\_p2frag$	0000344
15	reaction15		$C3 + XIAP\_p2frag\_C3 \rightleftharpoons C3 + BIR12\_C3 + BIR3R\_p2frag$	0000344
16	reaction16		$C3 + XIAP\_C9\_C3 \rightleftharpoons C3 + BIR12\_C3 + BIR3R\_C9$	0000344
17	reaction17		$C3 + XIAP\_2SMAC \rightleftharpoons C3 + BIR12\_SMAC + BIR3R\_SMAC$	0000344
18	reaction18		$C3 + XIAP\_C9\_C3 \rightleftharpoons C3 + C9P + XIAP\_p2frag\_C3$	0000344

№	Id	Name	Reaction Equation	SBO
19	reaction19		$C3 + XIAP\_C9 \rightleftharpoons C3 + C9P + XIAP\_p2frag$	0000344
20	reaction20		$C3 + BIR3R\_C9 \rightleftharpoons C3 + BIR3R\_p2frag + C9P$	0000344
21	reaction21		$C9 + XIAP \rightleftharpoons XIAP\_C9$	0000344
22	reaction22		$C9 + XIAP\_C3 \rightleftharpoons XIAP\_C9\_C3$	0000344
23	reaction23		$C9 + BIR3R \rightleftharpoons BIR3R\_C9$	0000344
24	reaction24		$BIR3R\_p2frag \rightleftharpoons BIR3R$	0000180
25	reaction25		$XIAP\_p2frag \rightleftharpoons XIAP$	0000180
26	reaction26		$XIAP + 2\,SMAC \rightleftharpoons XIAP\_2SMAC$	0000526
27	reaction27		$XIAP\_C9 + 2\,SMAC \rightleftharpoons XIAP\_2SMAC + C9$	0000526
28	reaction28		$XIAP\_C3 + 2\,SMAC \rightleftharpoons XIAP\_2SMAC + C3$	0000526
29	reaction29		$XIAP\_C9\_C3 + 2\,SMAC \rightleftharpoons XIAP\_2SMAC + C3 + C9$	0000526
30	reaction30		$BIR12 + SMAC \rightleftharpoons BIR12\_SMAC$	0000526
31	reaction31		$BIR3R + SMAC \rightleftharpoons BIR3R\_SMAC$	0000526
32	reaction32		$BIR12\_C3 + SMAC \rightleftharpoons BIR12\_SMAC + C3$	0000526
33	reaction33		$BIR3R\_C9 + SMAC \rightleftharpoons BIR3R\_SMAC + C9$	0000526
34	reaction34		$XIAP\_p2frag + 2\,SMAC \rightleftharpoons XIAP\_p2frag\_2SMAC$	0000526
35	reaction35		$C9P \rightleftharpoons \emptyset$	0000179
36	reaction36		$C9 \rightleftharpoons \emptyset$	0000179
37	reaction37		$C3 \rightleftharpoons \emptyset$	0000179
38	reaction38		$XIAP\_C3 \rightleftharpoons \emptyset$	0000179
39	reaction39		$XIAP\_C9\_C3 \rightleftharpoons \emptyset$	0000179
40	reaction40		$XIAP\_C9 \rightleftharpoons \emptyset$	0000179
41	reaction41		$XIAP\_p2frag \rightleftharpoons \emptyset$	0000179
42	reaction42		$XIAP\_p2frag\_C3 \rightleftharpoons \emptyset$	0000179
43	reaction43		$XIAP\_p2frag\_2SMAC \rightleftharpoons \emptyset$	0000179
44	reaction44		$XIAP\_2SMAC \rightleftharpoons \emptyset$	0000179
45	reaction45		$BIR12 \rightleftharpoons \emptyset$	0000179
46	reaction46		$BIR3R \rightleftharpoons \emptyset$	0000179

№	Id	Name	Reaction Equation	SBO
47	reaction47		BIR12_SMAC $\rightleftharpoons \emptyset$	0000179
48	reaction48		BIR3R_SMAC $\rightleftharpoons \emptyset$	0000179
49	reaction49		BIR12_C3 $\rightleftharpoons \emptyset$	0000179
50	reaction50		BIR3R_C9 $\rightleftharpoons \emptyset$	0000179
51	reaction51		BIR3R_p2frag $\rightleftharpoons \emptyset$	0000179
52	reaction52		SMAC $\rightleftharpoons \emptyset$	0000179
53	reaction53		C3 + Substrate $\rightleftharpoons$ C3 + ClvgPrds	0000344
54	SMAC_release		SMAC_mito $\rightleftharpoons$ SMAC	0000185
55	Apo_formation		PC9 + APAF1 $\rightleftharpoons$ C9	0000526
56	CytC_release		CytC_mit $\rightleftharpoons$ CytC_cell	0000185

9.1 Reaction `reaction1`

This is a reversible reaction of no reactant forming one product.

Name ProCaspase3 Production

SBO:0000393 production

Reaction equation

$$\emptyset \rightleftharpoons \mathrm{PC3} \tag{33}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
PC3	ProCasp3	

Kinetic Law

Derived unit $\mu\mathrm{mol} \cdot (60\ \mathrm{s})^{-1}$

$$v_1 = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k1} - \mathrm{k1r} \cdot [\mathrm{PC3}]) \tag{34}$$

9.2 Reaction `reaction2`

This is a reversible reaction of no reactant forming one product.

Name XIAP Production

SBO:0000393 production

Reaction equation

$$\emptyset \rightleftharpoons \mathrm{XIAP} \tag{35}$$

Product

Table 7: Properties of each product.

Id	Name	SBO
XIAP		

Kinetic Law

Derived unit $\mu\text{mol} \cdot (60\ \text{s})^{-1}$

$$v_2 = \text{vol}(\text{cell}) \cdot (\text{k2} - \text{k2r} \cdot [\text{XIAP}]) \tag{36}$$

9.3 Reaction `reaction3`

This is a reversible reaction of two reactants forming two products.

SBO:0000297 protein complex

Reaction equation

$$\text{C9} + \text{PC3} \rightleftharpoons \text{C3} + \text{C9} \tag{37}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
`C9`	Casp9(p35-p12)	
`PC3`	ProCasp3	

Products

Table 9: Properties of each product.

Id	Name	SBO
`C3`		
`C9`	Casp9(p35-p12)	

Kinetic Law

Derived unit $(60\ \text{s})^{-1} \cdot \mu\text{mol}$

$$v_3 = \text{vol}(\text{cell}) \cdot \text{k3} \cdot [\text{C9}] \cdot [\text{PC3}] \tag{38}$$

9.4 Reaction `reaction4`

This is a reversible reaction of two reactants forming two products.

SBO:0000231 occurring entity representation

Reaction equation

$$\mathrm{C9} + \mathrm{C3} \rightleftharpoons \mathrm{C9P} + \mathrm{C3} \tag{39}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
C9	Casp9(p35-p12)	
C3		

Products

Table 11: Properties of each product.

Id	Name	SBO
C9P	Casp9(p35-p10)	
C3		

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_4 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k4} \cdot [\mathrm{C9}] \cdot [\mathrm{C3}] \tag{40}$$

9.5 Reaction `reaction5`

This is a reversible reaction of two reactants forming two products.

SBO:0000231 occurring entity representation

Reaction equation

$$\mathrm{C9P} + \mathrm{PC3} \rightleftharpoons \mathrm{C9P} + \mathrm{C3} \tag{41}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
C9P	Casp9(p35-p10)	
PC3	ProCasp3	

Products

Table 13: Properties of each product.

Id	Name	SBO
C9P	Casp9(p35-p10)	
C3		

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_5 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k5} \cdot [\mathrm{C9P}] \cdot [\mathrm{PC3}] \tag{42}$$

9.6 Reaction reaction6

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

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{PC3} + \mathrm{C3} \rightleftharpoons 2\,\mathrm{C3} \tag{43}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
PC3	ProCasp3	
C3		

Product

Table 15: Properties of each product.

Id	Name	SBO
C3		

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_6 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k6} \cdot [\mathrm{PC3}] \cdot [\mathrm{C3}] \tag{44}$$

9.7 Reaction `reaction7`

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

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP} \rightleftharpoons \mathrm{XIAP\_C3} \tag{45}$$

Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
C3		
XIAP		

Product

Table 17: Properties of each product.

Id	Name	SBO
XIAP_C3	XIAP-Casp3	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_7 = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k7} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP}] - \mathrm{k7r} \cdot [\mathrm{XIAP\_C3}]) \tag{46}$$

9.8 Reaction `reaction8`

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

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP\_C9} \rightleftharpoons \mathrm{XIAP\_C9\_C3} \tag{47}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
C3		
XIAP_C9	XIAP-Casp9	

Product

Table 19: Properties of each product.

Id	Name	SBO
XIAP_C9_C3	XIAP-Casp9-Casp3	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_8 = \mathrm{vol}(\mathrm{cell}) \cdot (\mathrm{k8} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP\_C9}] - \mathrm{k8r} \cdot [\mathrm{XIAP\_C9\_C3}]) \tag{48}$$

9.9 Reaction reaction9

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

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP\_p2frag} \rightleftharpoons \mathrm{XIAP\_p2frag\_C3} \tag{49}$$

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
C3		
XIAP_p2frag	XIAP-p2 fragment	

Product

Table 21: Properties of each product.

Id	Name	SBO
XIAP_p2frag_C3	XIAP-p2frag-Casp3	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_9 = \mathrm{vol}(\mathrm{cell}) \cdot (\mathrm{k9} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP\_p2frag}] - \mathrm{k9r} \cdot [\mathrm{XIAP\_p2frag\_C3}]) \tag{50}$$

9.10 Reaction reaction10

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

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{C3} + \mathrm{BIR12} \rightleftharpoons \mathrm{BIR12\_C3} \tag{51}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
C3		
BIR12		

Product

Table 23: Properties of each product.

Id	Name	SBO
BIR12_C3	BIR12-Casp3	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{10} = \mathrm{vol}(\mathrm{cell}) \cdot (\mathrm{k10} \cdot [\mathrm{C3}] \cdot [\mathrm{BIR12}] - \mathrm{k10r} \cdot [\mathrm{BIR12\_C3}]) \tag{52}$$

9.11 Reaction `reaction11`

This is a reversible reaction of two reactants forming three products.

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP} \rightleftharpoons \mathrm{BIR12} + \mathrm{BIR3R} + \mathrm{C3} \tag{53}$$

Reactants

Table 24: Properties of each reactant.

Id	Name	SBO
C3		
XIAP		

Products

Table 25: Properties of each product.

Id	Name	SBO
BIR12		
BIR3R		
C3		

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{11} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k11} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP}] \tag{54}$$

9.12 Reaction `reaction12`

This is a reversible reaction of two reactants forming three products.

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP\_C9} \rightleftharpoons \mathrm{BIR12} + \mathrm{BIR3R\_C9} + \mathrm{C3} \tag{55}$$

Reactants

Table 26: Properties of each reactant.

Id	Name	SBO
C3		
XIAP_C9	XIAP-Casp9	

Products

Table 27: Properties of each product.

Id	Name	SBO
BIR12		
BIR3R_C9	BIR3R-Casp9	
C3		

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{12} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k12} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP\_C9}] \tag{56}$$

9.13 Reaction `reaction13`

This is a reversible reaction of two reactants forming three products.

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP\_C3} \rightleftharpoons \mathrm{C3} + \mathrm{BIR12\_C3} + \mathrm{BIR3R} \tag{57}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
C3		
XIAP_C3	XIAP-Casp3	

Products

Table 29: Properties of each product.

Id	Name	SBO
C3		
BIR12_C3	BIR12-Casp3	
BIR3R		

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{13} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k13} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP\_C3}] \tag{58}$$

9.14 Reaction reaction14

This is a reversible reaction of two reactants forming three products.

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP\_p2frag} \rightleftharpoons \mathrm{C3} + \mathrm{BIR12} + \mathrm{BIR3R\_p2frag} \tag{59}$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
C3		
XIAP_p2frag	XIAP-p2 fragment	

Products

Table 31: Properties of each product.

Id	Name	SBO
C3		
BIR12		
BIR3R_p2frag	BIR3R-p2frag	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{14} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k14} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP\_p2frag}] \tag{60}$$

9.15 Reaction `reaction15`

This is a reversible reaction of two reactants forming three products.

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP\_p2frag\_C3} \rightleftharpoons \mathrm{C3} + \mathrm{BIR12\_C3} + \mathrm{BIR3R\_p2frag} \tag{61}$$

Reactants

Table 32: Properties of each reactant.

Id	Name	SBO
`C3`		
`XIAP_p2frag_C3`	XIAP-p2frag-Casp3	

Products

Table 33: Properties of each product.

Id	Name	SBO
`C3`		
`BIR12_C3`	BIR12-Casp3	
`BIR3R_p2frag`	BIR3R-p2frag	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{15} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k15} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP\_p2frag\_C3}] \tag{62}$$

9.16 Reaction `reaction16`

This is a reversible reaction of two reactants forming three products.

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP\_C9\_C3} \rightleftharpoons \mathrm{C3} + \mathrm{BIR12\_C3} + \mathrm{BIR3R\_C9} \tag{63}$$

Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
C3		
XIAP_C9_C3	XIAP-Casp9-Casp3	

Products

Table 35: Properties of each product.

Id	Name	SBO
C3		
BIR12_C3	BIR12-Casp3	
BIR3R_C9	BIR3R-Casp9	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{16} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k16} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP\_C9\_C3}] \tag{64}$$

9.17 Reaction reaction17

This is a reversible reaction of two reactants forming three products.

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP\_2SMAC} \rightleftharpoons \mathrm{C3} + \mathrm{BIR12\_SMAC} + \mathrm{BIR3R\_SMAC} \tag{65}$$

Reactants

Table 36: Properties of each reactant.

Id	Name	SBO
C3		
XIAP_2SMAC	XIAP-2*SMAC	

Products

Table 37: Properties of each product.

Id	Name	SBO
C3		
BIR12_SMAC	BIR12-SMAC	
BIR3R_SMAC	BIR3R-SMAC	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{17} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k17} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP\_2SMAC}] \tag{66}$$

9.18 Reaction reaction18

This is a reversible reaction of two reactants forming three products.

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP\_C9\_C3} \rightleftharpoons \mathrm{C3} + \mathrm{C9P} + \mathrm{XIAP\_p2frag\_C3} \tag{67}$$

Reactants

Table 38: Properties of each reactant.

Id	Name	SBO
C3		
XIAP_C9_C3	XIAP-Casp9-Casp3	

Products

Table 39: Properties of each product.

Id	Name	SBO
C3		
C9P	Casp9(p35-p10)	
XIAP_p2frag_C3	XIAP-p2frag-Casp3	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{18} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k18} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP\_C9\_C3}] \tag{68}$$

9.19 Reaction reaction19

This is a reversible reaction of two reactants forming three products.

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C3} + \mathrm{XIAP\_C9} \rightleftharpoons \mathrm{C3} + \mathrm{C9P} + \mathrm{XIAP\_p2frag} \tag{69}$$

Reactants

Table 40: Properties of each reactant.

Id	Name	SBO
C3		
XIAP_C9	XIAP-Casp9	

Products

Table 41: Properties of each product.

Id	Name	SBO
C3		
C9P	Casp9(p35-p10)	
XIAP_p2frag	XIAP-p2 fragment	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{19} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k19} \cdot [\mathrm{C3}] \cdot [\mathrm{XIAP\_C9}] \tag{70}$$

9.20 Reaction `reaction20`

This is a reversible reaction of two reactants forming three products.

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C3} + \mathrm{BIR3R\_C9} \rightleftharpoons \mathrm{C3} + \mathrm{BIR3R\_p2frag} + \mathrm{C9P} \tag{71}$$

Reactants

Table 42: Properties of each reactant.

Id	Name	SBO
`C3`		
`BIR3R_C9`	BIR3R-Casp9	

Products

Table 43: Properties of each product.

Id	Name	SBO
`C3`		
`BIR3R_p2frag`	BIR3R-p2frag	
`C9P`	Casp9(p35-p10)	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{20} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k20} \cdot [\mathrm{C3}] \cdot [\mathrm{BIR3R\_C9}] \tag{72}$$

9.21 Reaction `reaction21`

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

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C9} + \mathrm{XIAP} \rightleftharpoons \mathrm{XIAP\_C9} \tag{73}$$

Reactants

Table 44: Properties of each reactant.

Id	Name	SBO
C9	Casp9(p35-p12)	
XIAP		

Product

Table 45: Properties of each product.

Id	Name	SBO
XIAP_C9	XIAP-Casp9	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{21} = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k21} \cdot [\mathrm{C9}] \cdot [\mathrm{XIAP}] - \mathrm{k21r} \cdot [\mathrm{XIAP\_C9}]) \tag{74}$$

9.22 Reaction reaction22

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

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C9} + \mathrm{XIAP\_C3} \rightleftharpoons \mathrm{XIAP\_C9\_C3} \tag{75}$$

Reactants

Table 46: Properties of each reactant.

Id	Name	SBO
C9	Casp9(p35-p12)	
XIAP_C3	XIAP-Casp3	

Product

Table 47: Properties of each product.

Id	Name	SBO
XIAP_C9_C3	XIAP-Casp9-Casp3	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{22} = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k22} \cdot [\mathrm{C9}] \cdot [\mathrm{XIAP\_C3}] - \mathrm{k22r} \cdot [\mathrm{XIAP\_C9\_C3}]) \tag{76}$$

9.23 Reaction reaction23

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

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C9} + \mathrm{BIR3R} \rightleftharpoons \mathrm{BIR3R\_C9} \tag{77}$$

Reactants

Table 48: Properties of each reactant.

Id	Name	SBO
C9	Casp9(p35-p12)	
BIR3R		

Product

Table 49: Properties of each product.

Id	Name	SBO
BIR3R_C9	BIR3R-Casp9	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{23} = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k23} \cdot [\mathrm{C9}] \cdot [\mathrm{BIR3R}] - \mathrm{k23r} \cdot [\mathrm{BIR3R\_C9}]) \tag{78}$$

9.24 Reaction `reaction24`

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

SBO:0000180 dissociation

Reaction equation

$$\mathrm{BIR3R\_p2frag} \rightleftharpoons \mathrm{BIR3R} \tag{79}$$

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
`BIR3R_p2frag`	BIR3R-p2frag	

Product

Table 51: Properties of each product.

Id	Name	SBO
`BIR3R`		

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k24} \cdot [\mathrm{BIR3R\_p2frag}] \tag{80}$$

9.25 Reaction `reaction25`

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

SBO:0000180 dissociation

Reaction equation

$$\mathrm{XIAP\_p2frag} \rightleftharpoons \mathrm{XIAP} \tag{81}$$

Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
XIAP_p2frag	XIAP-p2 fragment	

Product

Table 53: Properties of each product.

Id	Name	SBO
XIAP		

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k25} \cdot [\mathrm{XIAP\_p2frag}] \tag{82}$$

9.26 Reaction reaction26

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

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{XIAP} + 2\,\mathrm{SMAC} \rightleftharpoons \mathrm{XIAP\_2SMAC} \tag{83}$$

Reactants

Table 54: Properties of each reactant.

Id	Name	SBO
XIAP		
SMAC		

Product

Table 55: Properties of each product.

Id	Name	SBO
XIAP_2SMAC	XIAP-2*SMAC	

Id	Name	SBO

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{26} = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k26} \cdot [\mathrm{XIAP}] \cdot [\mathrm{SMAC}] \cdot [\mathrm{SMAC}] - \mathrm{k26r} \cdot [\mathrm{XIAP\_2SMAC}]) \quad (84)$$

9.27 Reaction `reaction27`

This is a reversible reaction of two reactants forming two products.

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{XIAP\_C9} + 2\,\mathrm{SMAC} \rightleftharpoons \mathrm{XIAP\_2SMAC} + \mathrm{C9} \quad (85)$$

Reactants

Table 56: Properties of each reactant.

Id	Name	SBO
`XIAP_C9`	XIAP-Casp9	
`SMAC`		

Products

Table 57: Properties of each product.

Id	Name	SBO
`XIAP_2SMAC`	XIAP-2*SMAC	
`C9`	Casp9(p35-p12)	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{27} = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k27} \cdot [\mathrm{XIAP\_C9}] \cdot [\mathrm{SMAC}] \cdot [\mathrm{SMAC}] - \mathrm{k27r} \cdot [\mathrm{XIAP\_2SMAC}] \cdot [\mathrm{C9}]) \quad (86)$$

9.28 Reaction `reaction28`

This is a reversible reaction of two reactants forming two products.

SBO:0000526 protein complex formation

Reaction equation

$$\text{XIAP\_C3} + 2\,\text{SMAC} \rightleftharpoons \text{XIAP\_2SMAC} + \text{C3} \tag{87}$$

Reactants

Table 58: Properties of each reactant.

Id	Name	SBO
XIAP_C3	XIAP-Casp3	
SMAC		

Products

Table 59: Properties of each product.

Id	Name	SBO
XIAP_2SMAC	XIAP-2*SMAC	
C3		

Kinetic Law

Derived unit $(60\ \text{s})^{-1} \cdot \mu\text{mol}$

$$v_{28} = \text{vol}(\text{cell}) \cdot (\text{k28} \cdot [\text{XIAP\_C3}] \cdot [\text{SMAC}] \cdot [\text{SMAC}] - \text{k28r} \cdot [\text{XIAP\_2SMAC}] \cdot [\text{C3}]) \tag{88}$$

9.29 Reaction reaction29

This is a reversible reaction of two reactants forming three products.

SBO:0000526 protein complex formation

Reaction equation

$$\text{XIAP\_C9\_C3} + 2\,\text{SMAC} \rightleftharpoons \text{XIAP\_2SMAC} + \text{C3} + \text{C9} \tag{89}$$

Reactants

Table 60: Properties of each reactant.

Id	Name	SBO
XIAP_C9_C3	XIAP-Casp9-Casp3	
SMAC		

Products

Table 61: Properties of each product.

Id	Name	SBO
XIAP_2SMAC	XIAP-2*SMAC	
C3		
C9	Casp9(p35-p12)	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{29} = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k29} \cdot [\mathrm{XIAP\_C9\_C3}] \cdot [\mathrm{SMAC}] \cdot [\mathrm{SMAC}] - \mathrm{k29r} \cdot [\mathrm{XIAP\_2SMAC}] \cdot [\mathrm{C3}] \cdot [\mathrm{C9}]) \tag{90}$$

9.30 Reaction reaction30

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

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{BIR12} + \mathrm{SMAC} \rightleftharpoons \mathrm{BIR12\_SMAC} \tag{91}$$

Reactants

Table 62: Properties of each reactant.

Id	Name	SBO
BIR12		
SMAC		

Product

Table 63: Properties of each product.

Id	Name	SBO
BIR12_SMAC	BIR12-SMAC	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{30} = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k30} \cdot [\mathrm{BIR12}] \cdot [\mathrm{SMAC}] - \mathrm{k30r} \cdot [\mathrm{BIR12\_SMAC}]) \tag{92}$$

9.31 Reaction reaction31

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

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{BIR3R} + \mathrm{SMAC} \rightleftharpoons \mathrm{BIR3R\_SMAC} \tag{93}$$

Reactants

Table 64: Properties of each reactant.

Id	Name	SBO
BIR3R		
SMAC		

Product

Table 65: Properties of each product.

Id	Name	SBO
BIR3R_SMAC	BIR3R-SMAC	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{31} = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k31} \cdot [\mathrm{BIR3R}] \cdot [\mathrm{SMAC}] - \mathrm{k31r} \cdot [\mathrm{BIR3R\_SMAC}]) \tag{94}$$

9.32 Reaction reaction32

This is a reversible reaction of two reactants forming two products.

SBO:0000526 protein complex formation

Reaction equation

$$\text{BIR12\_C3} + \text{SMAC} \rightleftharpoons \text{BIR12\_SMAC} + \text{C3} \tag{95}$$

Reactants

Table 66: Properties of each reactant.

Id	Name	SBO
BIR12_C3	BIR12-Casp3	
SMAC		

Products

Table 67: Properties of each product.

Id	Name	SBO
BIR12_SMAC	BIR12-SMAC	
C3		

Kinetic Law

Derived unit $(60\ \text{s})^{-1} \cdot \mu\text{mol}$

$$v_{32} = \text{vol}(\text{cell}) \cdot (\text{k32} \cdot [\text{BIR12\_C3}] \cdot [\text{SMAC}] - \text{k32r} \cdot [\text{BIR12\_SMAC}] \cdot [\text{C3}]) \tag{96}$$

9.33 Reaction reaction33

This is a reversible reaction of two reactants forming two products.

SBO:0000526 protein complex formation

Reaction equation

$$\text{BIR3R\_C9} + \text{SMAC} \rightleftharpoons \text{BIR3R\_SMAC} + \text{C9} \tag{97}$$

Reactants

Table 68: Properties of each reactant.

Id	Name	SBO
BIR3R_C9	BIR3R-Casp9	
SMAC		

Products

Table 69: Properties of each product.

Id	Name	SBO
BIR3R_SMAC	BIR3R-SMAC	
C9	Casp9(p35-p12)	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{33} = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k33} \cdot [\mathrm{BIR3R\_C9}] \cdot [\mathrm{SMAC}] - \mathrm{k33r} \cdot [\mathrm{BIR3R\_SMAC}] \cdot [\mathrm{C9}]) \quad (98)$$

9.34 Reaction reaction34

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

SBO:0000526 protein complex formation

Reaction equation

$$\mathrm{XIAP\_p2frag} + 2\,\mathrm{SMAC} \rightleftharpoons \mathrm{XIAP\_p2frag\_2SMAC} \quad (99)$$

Reactants

Table 70: Properties of each reactant.

Id	Name	SBO
XIAP_p2frag	XIAP-p2 fragment	
SMAC		

Product

Table 71: Properties of each product.

Id	Name	SBO
XIAP_p2frag_2SMAC	XIAP-p2frag-2*SMAC	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{34} = \mathrm{vol}(\mathrm{cell}) \cdot (\mathrm{k34} \cdot [\mathrm{XIAP\_p2frag}] \cdot [\mathrm{SMAC}] \cdot [\mathrm{SMAC}] - \mathrm{k34r} \cdot [\mathrm{XIAP\_p2frag\_2SMAC}]) \tag{100}$$

9.35 Reaction reaction35

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{C9P} \rightleftharpoons \emptyset \tag{101}$$

Reactant

Table 72: Properties of each reactant.

Id	Name	SBO
C9P	Casp9(p35-p10)	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{35} = \mathrm{vol}(\mathrm{cell}) \cdot \mathrm{k35} \cdot [\mathrm{C9P}] \tag{102}$$

9.36 Reaction reaction36

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{C9} \rightleftharpoons \emptyset \tag{103}$$

Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
C9	Casp9(p35-p12)	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{36} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k36} \cdot [\mathrm{C9}] \tag{104}$$

9.37 Reaction reaction37

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{C3} \rightleftharpoons \emptyset \tag{105}$$

Reactant

Table 74: Properties of each reactant.

Id	Name	SBO
C3		

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{37} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k37} \cdot [\mathrm{C3}] \tag{106}$$

9.38 Reaction reaction38

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\text{XIAP\_C3} \rightleftharpoons \emptyset \tag{107}$$

Reactant

Table 75: Properties of each reactant.

Id	Name	SBO
XIAP_C3	XIAP-Casp3	

Kinetic Law

Derived unit $(60\ \text{s})^{-1} \cdot \mu\text{mol}$

$$v_{38} = \text{vol}(\text{cell}) \cdot \text{k38} \cdot [\text{XIAP\_C3}] \tag{108}$$

9.39 Reaction reaction39

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\text{XIAP\_C9\_C3} \rightleftharpoons \emptyset \tag{109}$$

Reactant

Table 76: Properties of each reactant.

Id	Name	SBO
XIAP_C9_C3	XIAP-Casp9-Casp3	

Kinetic Law

Derived unit $(60\ \text{s})^{-1} \cdot \mu\text{mol}$

$$v_{39} = \text{vol}(\text{cell}) \cdot \text{k39} \cdot [\text{XIAP\_C9\_C3}] \tag{110}$$

9.40 Reaction reaction40

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\text{XIAP\_C9} \rightleftharpoons \emptyset \tag{111}$$

Reactant

Table 77: Properties of each reactant.

Id	Name	SBO
XIAP_C9	XIAP-Casp9	

Kinetic Law

Derived unit $(60\ \text{s})^{-1} \cdot \mu\text{mol}$

$$v_{40} = \text{vol}\,(\text{cell}) \cdot \text{k40} \cdot [\text{XIAP\_C9}] \tag{112}$$

9.41 Reaction reaction41

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\text{XIAP\_p2frag} \rightleftharpoons \emptyset \tag{113}$$

Reactant

Table 78: Properties of each reactant.

Id	Name	SBO
XIAP_p2frag	XIAP-p2 fragment	

Kinetic Law

Derived unit $(60\ \text{s})^{-1} \cdot \mu\text{mol}$

$$v_{41} = \text{vol}\,(\text{cell}) \cdot \text{k41} \cdot [\text{XIAP\_p2frag}] \tag{114}$$

9.42 Reaction reaction42

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\text{XIAP\_p2frag\_C3} \rightleftharpoons \emptyset \tag{115}$$

Reactant

Table 79: Properties of each reactant.

Id	Name	SBO
XIAP_p2frag_C3	XIAP-p2frag-Casp3	

Kinetic Law

Derived unit $(60\ \text{s})^{-1} \cdot \mu\text{mol}$

$$v_{42} = \text{vol}\,(\text{cell}) \cdot \text{k42} \cdot [\text{XIAP\_p2frag\_C3}] \tag{116}$$

9.43 Reaction reaction43

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\text{XIAP\_p2frag\_2SMAC} \rightleftharpoons \emptyset \tag{117}$$

Reactant

Table 80: Properties of each reactant.

Id	Name	SBO
XIAP_p2frag_2SMAC	XIAP-p2frag-2*SMAC	

Kinetic Law

Derived unit $(60\ \text{s})^{-1} \cdot \mu\text{mol}$

$$v_{43} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k43} \cdot [\mathrm{XIAP\_p2frag\_2SMAC}] \tag{118}$$

9.44 Reaction `reaction44`

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{XIAP\_2SMAC} \rightleftharpoons \emptyset \tag{119}$$

Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
`XIAP_2SMAC`	XIAP-2*SMAC	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{44} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k44} \cdot [\mathrm{XIAP\_2SMAC}] \tag{120}$$

9.45 Reaction `reaction45`

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{BIR12} \rightleftharpoons \emptyset \tag{121}$$

Reactant

Table 82: Properties of each reactant.

Id	Name	SBO
`BIR12`		

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{45} = \mathrm{vol}(\mathrm{cell}) \cdot \mathrm{k45} \cdot [\mathrm{BIR12}] \tag{122}$$

9.46 Reaction `reaction46`

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{BIR3R} \rightleftharpoons \emptyset \tag{123}$$

Reactant

Table 83: Properties of each reactant.

Id	Name	SBO
BIR3R		

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{46} = \mathrm{vol}(\mathrm{cell}) \cdot \mathrm{k46} \cdot [\mathrm{BIR3R}] \tag{124}$$

9.47 Reaction `reaction47`

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{BIR12\_SMAC} \rightleftharpoons \emptyset \tag{125}$$

Reactant

Table 84: Properties of each reactant.

Id	Name	SBO
BIR12_SMAC	BIR12-SMAC	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{47} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k47} \cdot [\mathrm{BIR12\_SMAC}] \tag{126}$$

9.48 Reaction reaction48

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{BIR3R\_SMAC} \rightleftharpoons \emptyset \tag{127}$$

Reactant

Table 85: Properties of each reactant.

Id	Name	SBO
BIR3R_SMAC	BIR3R-SMAC	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{48} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k48} \cdot [\mathrm{BIR3R\_SMAC}] \tag{128}$$

9.49 Reaction reaction49

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{BIR12\_C3} \rightleftharpoons \emptyset \tag{129}$$

Reactant

Table 86: Properties of each reactant.

Id	Name	SBO
BIR12_C3	BIR12-Casp3	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{49} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k49} \cdot [\mathrm{BIR12\_C3}] \tag{130}$$

9.50 Reaction reaction50

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{BIR3R\_C9} \rightleftharpoons \emptyset \tag{131}$$

Reactant

Table 87: Properties of each reactant.

Id	Name	SBO
BIR3R_C9	BIR3R-Casp9	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{50} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k50} \cdot [\mathrm{BIR3R\_C9}] \tag{132}$$

9.51 Reaction reaction51

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\text{BIR3R\_p2frag} \rightleftharpoons \emptyset \tag{133}$$

Reactant

Table 88: Properties of each reactant.

Id	Name	SBO
BIR3R_p2frag	BIR3R-p2frag	

Kinetic Law

Derived unit $(60\ \text{s})^{-1} \cdot \mu\text{mol}$

$$v_{51} = \text{vol}(\text{cell}) \cdot \text{k51} \cdot [\text{BIR3R\_p2frag}] \tag{134}$$

9.52 Reaction reaction52

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\text{SMAC} \rightleftharpoons \emptyset \tag{135}$$

Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
SMAC		

Kinetic Law

Derived unit $(60\ \text{s})^{-1} \cdot \mu\text{mol}$

$$v_{52} = \text{vol}(\text{cell}) \cdot \text{k52} \cdot [\text{SMAC}] \tag{136}$$

9.53 Reaction reaction53

This is a reversible reaction of two reactants forming two products.

SBO:0000344 molecular interaction

Reaction equation

$$\mathrm{C3} + \mathrm{Substrate} \rightleftharpoons \mathrm{C3} + \mathrm{ClvgPrds} \tag{137}$$

Reactants

Table 90: Properties of each reactant.

Id	Name	SBO
C3		
Substrate	Casp3 Substrate	

Products

Table 91: Properties of each product.

Id	Name	SBO
C3		
ClvgPrds	Clevage Products	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_{53} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k53} \cdot [\mathrm{C3}] \cdot [\mathrm{Substrate}] \tag{138}$$

9.54 Reaction SMAC_release

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

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{SMAC\_mito} \rightleftharpoons \mathrm{SMAC} \tag{139}$$

Reactant

Table 92: Properties of each reactant.

Id	Name	SBO
SMAC_mito	SMAC in mitochondrium	

Product

Table 93: Properties of each product.

Id	Name	SBO
SMAC		

Kinetic Law

Derived unit $\mu\text{mol} \cdot (60\ \text{s})^{-1}$

$$v_{54} = \frac{\text{vol}\,(\text{cell}) \cdot [\text{SMAC\_mito}] \cdot \ln 2}{\text{th\_SMAC}} \tag{140}$$

9.55 Reaction Apo_formation

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

SBO:0000526 protein complex formation

Reaction equation

$$\text{PC9} + \text{APAF1} \rightleftharpoons \text{C9} \tag{141}$$

Reactants

Table 94: Properties of each reactant.

Id	Name	SBO
PC9	ProCasp9	
APAF1		

Product

Table 95: Properties of each product.

Id	Name	SBO
C9	Casp9(p35-p12)	

Kinetic Law

Derived unit $\mu\text{mol} \cdot (60\ \text{s})^{-1}$

$$v_{55} = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{apo\_lim} \cdot \ln 2}{\mathrm{th\_Apop}} \tag{142}$$

9.56 Reaction `CytC_release`

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

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{CytC\_mit} \rightleftharpoons \mathrm{CytC\_cell} \tag{143}$$

Reactant

Table 96: Properties of each reactant.

Id	Name	SBO
`CytC_mit`	Cytochrome C in mitochondrium	

Product

Table 97: Properties of each product.

Id	Name	SBO
`CytC_cell`	cytosolic Cytochrome C	

Kinetic Law

Derived unit $\mu\mathrm{mol} \cdot (60\ \mathrm{s})^{-1}$

$$v_{56} = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{CytC\_mit}] \cdot \ln 2}{\mathrm{th\_CytC}} \tag{144}$$

10 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.

10.1 Species PC3

Name ProCasp3

SBO:0000245 macromolecule

Initial concentration $0.12\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in reaction3, reaction5, reaction6 and as a product in reaction1).

$$\frac{\text{d}}{\text{d}t}\text{PC3} = v_1 - v_3 - v_5 - v_6 \tag{145}$$

10.2 Species XIAP

SBO:0000245 macromolecule

Initial concentration $0.063\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in reaction7, reaction11, reaction21, reaction26 and as a product in reaction2, reaction25).

$$\frac{\text{d}}{\text{d}t}\text{XIAP} = v_2 + v_{25} - v_7 - v_{11} - v_{21} - v_{26} \tag{146}$$

10.3 Species C9

Name Casp9(p35-p12)

SBO:0000245 macromolecule

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

This species takes part in eleven reactions (as a reactant in reaction3, reaction4, reaction21, reaction22, reaction23, reaction36 and as a product in reaction3, reaction27, reaction29, reaction33, Apo_formation).

$$\frac{\text{d}}{\text{d}t}\text{C9} = v_3 + v_{27} + v_{29} + v_{33} + v_{55} - v_3 - v_4 - v_{21} - v_{22} - v_{23} - v_{36} \tag{147}$$

10.4 Species PC9

Name ProCasp9

SBO:0000245 macromolecule

Initial concentration $0.03\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PC9} = -v_{55} \tag{148}$$

10.5 Species C3

SBO:0000245 macromolecule

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

This species takes part in 36 reactions (as a reactant in reaction4, reaction6, reaction7, reaction8, reaction9, reaction10, reaction11, reaction12, reaction13, reaction14, reaction15, reaction16, reaction17, reaction18, reaction19, reaction20, reaction37, reaction53 and as a product in reaction3, reaction4, reaction5, reaction6, reaction11, reaction12, reaction13, reaction14, reaction15, reaction16, reaction17, reaction18, reaction19, reaction20, reaction28, reaction29, reaction32, reaction53).

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C3} = {} & v_3 + v_4 + v_5 + 2v_6 + v_{11} + v_{12} + v_{13} + v_{14} + v_{15} + v_{16} + v_{17} + v_{18} \\ & + v_{19} + v_{20} + v_{28} + v_{29} + v_{32} + v_{53} - v_4 - v_6 - v_7 - v_8 - v_9 - v_{10} \\ & - v_{11} - v_{12} - v_{13} - v_{14} - v_{15} - v_{16} - v_{17} - v_{18} - v_{19} - v_{20} - v_{37} - v_{53}\end{aligned} \tag{149}$$

10.6 Species C9P

Name Casp9(p35-p10)

SBO:0000245 macromolecule

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

This species takes part in seven reactions (as a reactant in reaction5, reaction35 and as a product in reaction4, reaction5, reaction18, reaction19, reaction20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C9P} = v_4 + v_5 + v_{18} + v_{19} + v_{20} - v_5 - v_{35} \tag{150}$$

10.7 Species XIAP_C3

Name XIAP-Casp3

SBO:0000296 macromolecular complex

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

This species takes part in five reactions (as a reactant in reaction13, reaction22, reaction28, reaction38 and as a product in reaction7).

$$\frac{\text{d}}{\text{d}t}\text{XIAP\_C3} = v_7 - v_{13} - v_{22} - v_{28} - v_{38} \tag{151}$$

10.8 Species XIAP_C9

Name XIAP-Casp9

SBO:0000296 macromolecular complex

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

This species takes part in six reactions (as a reactant in reaction8, reaction12, reaction19, reaction27, reaction40 and as a product in reaction21).

$$\frac{\text{d}}{\text{d}t}\text{XIAP\_C9} = v_{21} - v_8 - v_{12} - v_{19} - v_{27} - v_{40} \tag{152}$$

10.9 Species XIAP_C9_C3

Name XIAP-Casp9-Casp3

SBO:0000296 macromolecular complex

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

This species takes part in six reactions (as a reactant in reaction16, reaction18, reaction29, reaction39 and as a product in reaction8, reaction22).

$$\frac{\text{d}}{\text{d}t}\text{XIAP\_C9\_C3} = v_8 + v_{22} - v_{16} - v_{18} - v_{29} - v_{39} \tag{153}$$

10.10 Species XIAP_p2frag

Name XIAP-p2 fragment

SBO:0000296 macromolecular complex

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

This species takes part in six reactions (as a reactant in reaction9, reaction14, reaction25, reaction34, reaction41 and as a product in reaction19).

$$\frac{\text{d}}{\text{d}t}\text{XIAP\_p2frag} = v_{19} - v_9 - v_{14} - v_{25} - v_{34} - v_{41} \tag{154}$$

10.11 Species XIAP_p2frag_C3

Name XIAP-p2frag-Casp3

SBO:0000296 macromolecular complex

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

This species takes part in four reactions (as a reactant in reaction15, reaction42 and as a product in reaction9, reaction18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{XIAP\_p2frag\_C3} = v_9 + v_{18} - v_{15} - v_{42} \tag{155}$$

10.12 Species BIR12

SBO:0000245 macromolecule

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

This species takes part in six reactions (as a reactant in reaction10, reaction30, reaction45 and as a product in reaction11, reaction12, reaction14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{BIR12} = v_{11} + v_{12} + v_{14} - v_{10} - v_{30} - v_{45} \tag{156}$$

10.13 Species BIR12_C3

Name BIR12-Casp3

SBO:0000296 macromolecular complex

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

This species takes part in six reactions (as a reactant in reaction32, reaction49 and as a product in reaction10, reaction13, reaction15, reaction16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{BIR12\_C3} = v_{10} + v_{13} + v_{15} + v_{16} - v_{32} - v_{49} \tag{157}$$

10.14 Species BIR3R

SBO:0000245 macromolecule

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

This species takes part in six reactions (as a reactant in reaction23, reaction31, reaction46 and as a product in reaction11, reaction13, reaction24).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{BIR3R} = v_{11} + v_{13} + v_{24} - v_{23} - v_{31} - v_{46} \tag{158}$$

10.15 Species BIR3R_C9

Name BIR3R-Casp9

SBO:0000296 macromolecular complex

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

This species takes part in six reactions (as a reactant in reaction20, reaction33, reaction50 and as a product in reaction12, reaction16, reaction23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{BIR3R\_C9} = v_{12} + v_{16} + v_{23} - v_{20} - v_{33} - v_{50} \tag{159}$$

10.16 Species BIR3R_p2frag

Name BIR3R-p2frag

SBO:0000296 macromolecular complex

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

This species takes part in five reactions (as a reactant in reaction24, reaction51 and as a product in reaction14, reaction15, reaction20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{BIR3R\_p2frag} = v_{14} + v_{15} + v_{20} - v_{24} - v_{51} \tag{160}$$

10.17 Species XIAP_2SMAC

Name XIAP-2*SMAC

SBO:0000296 macromolecular complex

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

This species takes part in six reactions (as a reactant in reaction17, reaction44 and as a product in reaction26, reaction27, reaction28, reaction29).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{XIAP\_2SMAC} = v_{26} + v_{27} + v_{28} + v_{29} - v_{17} - v_{44} \tag{161}$$

10.18 Species BIR12_SMAC

Name BIR12-SMAC

SBO:0000296 macromolecular complex

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

This species takes part in four reactions (as a reactant in reaction47 and as a product in reaction17, reaction30, reaction32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{BIR12\_SMAC} = v_{17} + v_{30} + v_{32} - v_{47} \tag{162}$$

10.19 Species BIR3R_SMAC

Name BIR3R-SMAC

SBO:0000296 macromolecular complex

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

This species takes part in four reactions (as a reactant in reaction48 and as a product in reaction17, reaction31, reaction33).

$$\frac{\text{d}}{\text{d}t}\text{BIR3R\_SMAC} = v_{17} + v_{31} + v_{33} - v_{48} \tag{163}$$

10.20 Species SMAC

SBO:0000245 macromolecule

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

This species takes part in eleven reactions (as a reactant in reaction26, reaction27, reaction28, reaction29, reaction30, reaction31, reaction32, reaction33, reaction34, reaction52 and as a product in SMAC_release).

$$\frac{\text{d}}{\text{d}t}\text{SMAC} = v_{54} - 2v_{26} - 2v_{27} - 2v_{28} - 2v_{29} - v_{30} - v_{31} - v_{32} - v_{33} - 2v_{34} - v_{52} \tag{164}$$

10.21 Species APAF1

SBO:0000245 macromolecule

Initial concentration $3.372\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{APAF1} = -v_{55} \tag{165}$$

10.22 Species XIAP_p2frag_2SMAC

Name XIAP-p2frag-2*SMAC

SBO:0000296 macromolecular complex

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

This species takes part in two reactions (as a reactant in reaction43 and as a product in reaction34).

$$\frac{\text{d}}{\text{d}t}\text{XIAP\_p2frag\_2SMAC} = v_{34} - v_{43} \tag{166}$$

10.23 Species Substrate

Name Casp3 Substrate

SBO:0000252 polypeptide chain

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

This species takes part in one reaction (as a reactant in reaction53).

$$\frac{\text{d}}{\text{d}t}\text{Substrate} = -v_{53} \tag{167}$$

10.24 Species ClvgPrds

Name Clevage Products

SBO:0000252 polypeptide chain

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

This species takes part in one reaction (as a product in reaction53).

$$\frac{\text{d}}{\text{d}t}\text{ClvgPrds} = v_{53} \tag{168}$$

10.25 Species SMAC_mito

Name SMAC in mitochondrium

SBO:0000245 macromolecule

Initial concentration 0.126 $\mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{SMAC\_mito} = -v_{54} \tag{169}$$

10.26 Species CytC_mit

Name Cytochrome C in mitochondrium

SBO:0000245 macromolecule

Initial concentration 10 $\mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{CytC\_mit} = -v_{56} \tag{170}$$

10.27 Species CytC_cell

Name cytosolic Cytochrome C

SBO:0000245 macromolecule

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

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

$$\frac{\text{d}}{\text{d}t}\text{CytC\_cell} = v_{56} \tag{171}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000179 degradation: Complete disappearance of a physical entity

SBO:0000180 dissociation: Transformation of a non-covalent complex that results in the formation of several independent biochemical entitie

SBO:0000185 transport reaction: Movement of a physical entity without modification of the structure of the entity

SBO:0000231 occurring entity representation: Representation of an entity that manifests, unfolds or develops through time, such as a discrete event, or a mutual or reciprocal action or influence that happens between participating physical entities, and/or other occurring entities.

SBO:0000245 macromolecule: Molecular entity mainly built-up by the repetition of pseudo-identical units. CHEBI:3383

SBO:0000252 polypeptide chain: Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

SBO:0000296 macromolecular complex: Non-covalent complex of one or more macromolecules and zero or more simple chemicals

SBO:0000297 protein complex: Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608

SBO:0000344 molecular interaction: Relationship between molecular entities, based on contacts, direct or indirect.

SBO:0000393 production: Generation of a material or conceptual entity.

SBO:0000526 protein complex formation: The process by which two or more proteins interact non-covalently to form a protein complex (SBO:0000297)

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