SBML Model Report

Model name: “Kim2007 - Crosstalk between Wnt and ERK pathways”

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Harish Dharuri[1] and Vijayalakshmi Chelliah[2] at July tenth 2007 at 1:55 p. m. and last time modified at October 22nd 2014 at 12:15 a. 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	2
species types	0	species	28
events	2	constraints	0
reactions	33	function definitions	0
global parameters	59	unit definitions	2
rules	1	initial assignments	0

Model Notes

Kim2007 - Crosstalk between Wnt and ERK pathways

Experimental studies have shown that both Wnt and the MAPK pathways are involved in the pathogenesis of various kinds of cancers (eg. colorectal cancer). The crosstalk between the two pathways have also been identified. Here, Kim et al., (2007) have integrated the experimental

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evidences on crosstalk mechanisms between the two pathways into a pathway model, and have identified the existence of a hidden positive feedback loop and suggest that this positive feedback loop might participate in the pathogenesis of colorectal cancer.

This model is described in the article:A hidden oncogenic positive feedback loop caused by crosstalk between Wnt and ERK pathways.Kim D, Rath O, Kolch W, Cho KH.Oncogene 2007 Jul; 26(31): 4571-4579

Abstract:

The Wnt and the extracellular signal regulated-kinase (ERK) pathways are both involved in the pathogenesis of various kinds of cancers. Recently, the existence of crosstalk between Wnt and ERK pathways was reported. Gathering all reported results, we have discovered a positive feedback loop embedded in the crosstalk between the Wnt and ERK pathways. We have developed a plausible model that represents the role of this hidden positive feedback loop in the Wnt/ERK pathway crosstalk based on the integration of experimental reports and employing established basic mathematical models of each pathway. Our analysis shows that the positive feedback loop can generate bistability in both the Wnt and ERK signaling pathways, and this prediction was further validated by experiments. In particular, using the commonly accepted assumption that mutations in signaling proteins contribute to cancerogenesis, we have found two conditions through which mutations could evoke an irreversible response leading to a sustained activation of both pathways. One condition is enhanced production of beta-catenin, the other is a reduction of the velocity of MAP kinase phosphatase(s). This enables that high activities of Wnt and ERK pathways are maintained even without a persistent extracellular signal. Thus, our study adds a novel aspect to the molecular mechanisms of carcinogenesis by showing that mutational changes in individual proteins can cause fundamental functional changes well beyond the pathway they function in by a positive feedback loop embedded in crosstalk. Thus, crosstalk between signaling pathways provides a vehicle through which mutations of individual components can affect properties of the system at a larger scale.

Figure 6 of the reference publication has been reproduced. The model as such reproduces the plots corresponding to the normal conditions. To obtain simulations under 1) beta-cataenin mutation; set V12=0.846 (two-fold of the beta-catenin synthetic rate than the normal system. i.e. 2*0.426), 2) PP2A mutation; set Vmax4=Vmax5=33.75 (three-fourths of the PP2A activity that the normal system. i.e. (3/4)*45). The simulation was performed using Copasi 4.10 (Build 55).

This model is hosted on BioModels Database and identifiedby: BIOMD0000000149 .

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

2 Unit Definitions

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

2.1 Unit substance

Name nanomole

Definition nmol

2.2 Unit time

Name minute

Definition 60 s

2.3 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.4 Unit area

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

Definition m^2

2.5 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
cytoplasm	cytoplasm		3	1	litre	☑	
nucleus	nucleus		3	1	litre	☑	cytoplasm

3.1 Compartment cytoplasm

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

Name cytoplasm

3.2 Compartment `nucleus`

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

Name nucleus

4 Species

This model contains 28 species. Section 9 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
X1	Dshi	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X2	Dsha	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X3	APC_ast/Axin_ast/GSK3beta	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X4	APC/Axin/GSK3beta	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X5	GSK3beta	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X6	APC/Axin	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X7	APC	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X8	bCatenin/APC_Ast/Axin_ast/GSK3beta	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X9	bCatenin_ast/APC_ast/Axin-_ast/GSK3beta	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X10	bCatenin_ast	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X11	bCatenin	nucleus	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X12	Axin	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X13	TCF	nucleus	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X14	bCatenin/TCF	nucleus	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X15	bCatenin/APC	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X16	Rasi	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X17	Rasa	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X18	Raf-1	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X19	Raf-1_ast	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X20	MEK	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X21	MEK_ast	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
X22	ERK	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X23	ERK_ast	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X24	Raf1/RKIP	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X25	RKIP	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X26	RKIP_ast	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X27	unknown molecule X	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X28	GSK3beta	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 59 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.182		☑
W			0.000		☐
k2			0.018		☑
k3			0.050		☑
k4			0.267		☑
k5			0.133		☑
k_plus6			0.091		☑
k_minus6			0.909		☑
k_plus7			1.000		☑
k_minus7			50.000		☑
k_plus8			1.000		☑
k_minus8			120.000		☑
k9			206.000		☑
k10			206.000		☑
k11			0.417		☑
V12			0.423		☑
k13			$2.57 \cdot 10^{-4}$		☑
k14			$8.22 \cdot 10^{-5}$		☑
k21			10^{-6}		☑
k15			0.167		☑
k_plus16			1.000		☑
k_minus16			30.000		☑
k_plus17			1.000		☑
k_minus17			1200.000		☑
Vmax1			150.000		☑
Km1			10.000		☑
Ki			9.000		☑
Vmax2			15.000		☑
Km2			8.000		☑
kcat1			1.500		☑
Km3			15.000		☑
Vmax3			45.000		☑
Km4			15.000		☑
kcat2			1.500		☑
Km5			15.000		☑
Vmax4			45.000		☑
Km6			15.000		☑

Id	Name	SBO	Value	Unit	Constant
kcat3			1.500		☑
Km7			15.000		☑
Vmax5			45.000		☑
Km8			15.000		☑
kcat4			1.500		☑
Km9			9.000		☑
k18			0.150		☑
k19			39.000		☑
Vmax6			45.000		☑
Km10			12.000		☑
kcat5			0.600		☑
n1			2.000		☑
Km11			15.000		☑
k20			0.015		☑
kcat6			1.500		☑
Km12			15.000		☑
kcat7			1.500		☑
Km13			15.000		☑
Vmax7			45.000		☑
Km14			15.000		☑
flag_for-_wnt_signal			0.000		⊟
X13X14			0.000		⊟

6 Rule

This is an overview of one rule.

6.1 Rule X13X14

Rule X13X14 is an assignment rule for parameter X13X14:

$$\mathrm{X13X14} = [\mathrm{X13}] + [\mathrm{X14}] \tag{1}$$

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

7 Events

This is an overview of two events. 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.

7.1 Event event_0000001

Notes The two events are used to increase the value of wnt from 0 to 1 between time t=500minutes and t=1000minutes.

Trigger condition

$$(t \geq 500) \wedge (t \leq 1000) \tag{2}$$

Assignment

$$W = 1 \tag{3}$$

7.2 Event event_0000002

Trigger condition

$$t > 1000 \tag{4}$$

Assignment

$$W = 0 \tag{5}$$

8 Reactions

This model contains 33 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	R1	Dishevelled activation	$X1 \longrightarrow X2$	
2	R2	Dishevelled inactivation	$X2 \longrightarrow X1$	
3	R3	Dishevelled mediated GSK/Axin/APC complex disassembly	$X4 \xrightarrow{X2} X6 + X5$	
4	R4	Activation of GSK/Axin/APC complex	$X4 \longrightarrow X3$	
5	R5	Inactivation of GSK/Axin/APC complex	$X3 \longrightarrow X4$	
6	R6	GSK/Axin/APC complex reassembly	$X6 + X5 \rightleftharpoons X4$	
7	R7	Axin/APC complex formation	$X12 + X7 \rightleftharpoons X6$	
8	R8	bCatenin binding to GSK/Axin/APC complex	$X11 + X3 \rightleftharpoons X8$	
9	R9	bCatenin phosphorylation	$X8 \longrightarrow X9$	
10	R10	GSK.Axin/APC/bCatenin complex disassembly	$X9 \longrightarrow X3 + X10$	
11	R11	Phosphorylated bCatenin degradation	$X10 \longrightarrow \emptyset$	
12	R12	bCatenin synthesis	$\emptyset \longrightarrow X11$	
13	R13	Unphosphorylated bCatenin degradation	$X11 \longrightarrow \emptyset$	
14	R14	Axin synthesis	$\emptyset \xrightarrow{X11,\ X14} X12$	
15	R15	Axin degradation	$X12 \longrightarrow \emptyset$	
16	R16	bCatenin/TCF complex formation	$X13 + X11 \rightleftharpoons X14$	
17	R17	APC/bCatenin complex formation	$X11 + X7 \rightleftharpoons X15$	
18	R18	Ras activation	$X16 \xrightarrow{X23} X17$	
19	R19	Ras inactivation	$X17 \longrightarrow X16$	

№	Id	Name	Reaction Equation	SBO
20	R20	Raf activation	$X18 \xrightarrow{X17} X19$	
21	R21	Raf inactivation	$X19 \longrightarrow X18$	
22	R22	MEK activation	$X20 \xrightarrow{X19} X21$	
23	R23	MEK inactivation	$X21 \longrightarrow X20$	
24	R24	ERK activation	$X22 \xrightarrow{X21} X23$	
25	R25	ERK inactivation	$X23 \longrightarrow X22$	
26	R26	Raf/RKIP complex disassembly	$X24 \xrightarrow{X23} X18 + X26$	
27	R27	Raf-RKIP complex formation	$X18 + X25 \rightleftharpoons X24$	
28	R28	RKIP dephosphorylation	$X26 \longrightarrow X25$	
29	R29	Unknown factor-X formation	$\emptyset \xrightarrow{X14} X27$	
30	R30	Factor-X degradation	$X27 \longrightarrow \emptyset$	
31	R31	Factor-X mediated Raf activation	$X18 \xrightarrow{X27} X19$	
32	R32	ERK mediated GSK3beta phosphorylation	$X5 \xrightarrow{X23} X28$	
33	R33	GSK3beta dephosphorylation	$X28 \longrightarrow X5$	

8.1 Reaction R1

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

Name Dishevelled activation

Reaction equation

$$\mathrm{X1} \longrightarrow \mathrm{X2} \tag{6}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
X1	Dshi	

Product

Table 7: Properties of each product.

Id	Name	SBO
X2	Dsha	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k1} \cdot [\mathrm{X1}] \cdot \mathrm{W} \tag{7}$$

8.2 Reaction R2

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

Name Dishevelled inactivation

Reaction equation

$$\mathrm{X2} \longrightarrow \mathrm{X1} \tag{8}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
X2	Dsha	

Product

Table 9: Properties of each product.

Id	Name	SBO
X1	Dshi	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k2} \cdot [\mathrm{X2}] \tag{9}$$

8.3 Reaction R3

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

Name Dishevelled mediated GSK/Axin/APC complex disassembly

Reaction equation

$$\mathrm{X4} \xrightarrow{\mathrm{X2}} \mathrm{X6} + \mathrm{X5} \tag{10}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
X4	APC/Axin/GSK3beta	

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
X2	Dsha	

Products

Table 12: Properties of each product.

Id	Name	SBO
X6	APC/Axin	
X5	GSK3beta	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k3} \cdot [\mathrm{X2}] \cdot [\mathrm{X4}] \tag{11}$$

8.4 Reaction R4

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

Name Activation of GSK/Axin/APC complex

Reaction equation

$$\mathrm{X4} \longrightarrow \mathrm{X3} \tag{12}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
X4	APC/Axin/GSK3beta	

Product

Table 14: Properties of each product.

Id	Name	SBO
X3	APC_ast/Axin_ast/GSK3beta	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k4} \cdot [\mathrm{X4}] \tag{13}$$

8.5 Reaction R5

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

Name Inactivation of GSK/Axin/APC complex

Reaction equation

$$\mathrm{X3} \longrightarrow \mathrm{X4} \tag{14}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
X3	APC_ast/Axin_ast/GSK3beta	

Product

Table 16: Properties of each product.

Id	Name	SBO
X4	APC/Axin/GSK3beta	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k5} \cdot [\mathrm{X3}] \tag{15}$$

8.6 Reaction R6

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

Name GSK/Axin/APC complex reassembly

Reaction equation

$$\mathrm{X6} + \mathrm{X5} \rightleftharpoons \mathrm{X4} \tag{16}$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
X6	APC/Axin	
X5	GSK3beta	

Product

Table 18: Properties of each product.

Id	Name	SBO
X4	APC/Axin/GSK3beta	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot (\mathrm{k\_plus6} \cdot [\mathrm{X5}] \cdot [\mathrm{X6}] - \mathrm{k\_minus6} \cdot [\mathrm{X4}]) \tag{17}$$

8.7 Reaction R7

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

Name Axin/APC complex formation

Reaction equation

$$\mathrm{X12} + \mathrm{X7} \rightleftharpoons \mathrm{X6} \tag{18}$$

Reactants

Table 19: Properties of each reactant.

Id	Name	SBO
X12	Axin	
X7	APC	

Product

Table 20: Properties of each product.

Id	Name	SBO
X6	APC/Axin	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}(\mathrm{cytoplasm}) \cdot (\mathrm{k\_plus7} \cdot [\mathrm{X7}] \cdot [\mathrm{X12}] - \mathrm{k\_minus7} \cdot [\mathrm{X6}]) \tag{19}$$

8.8 Reaction R8

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

Name bCatenin binding to GSK/Axin/APC complex

Reaction equation

$$\mathrm{X11} + \mathrm{X3} \rightleftharpoons \mathrm{X8} \tag{20}$$

Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
X11	bCatenin	
X3	APC_ast/Axin_ast/GSK3beta	

Product

Table 22: Properties of each product.

Id	Name	SBO
X8	bCatenin/APC_Ast/Axin_ast/GSK3beta	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}(\mathrm{cytoplasm}) \cdot (\mathrm{k\_plus8} \cdot [\mathrm{X3}] \cdot [\mathrm{X11}] - \mathrm{k\_minus8} \cdot [\mathrm{X8}]) \tag{21}$$

8.9 Reaction R9

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

Name bCatenin phosphorylation

Reaction equation

$$\mathrm{X8} \longrightarrow \mathrm{X9} \tag{22}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
X8	bCatenin/APC_Ast/Axin_ast/GSK3beta	

Product

Table 24: Properties of each product.

Id	Name	SBO
X9	bCatenin_ast/APC_ast/Axin_ast/GSK3beta	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k9} \cdot [\mathrm{X8}] \tag{23}$$

8.10 Reaction R10

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

Name GSK.Axin/APC/bCatenin complex disassembly

Reaction equation

$$\mathrm{X9} \longrightarrow \mathrm{X3} + \mathrm{X10} \tag{24}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
X9	bCatenin_ast/APC_ast/Axin_ast/GSK3beta	

Products

Table 26: Properties of each product.

Id	Name	SBO
X3	APC_ast/Axin_ast/GSK3beta	
X10	bCatenin_ast	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k10} \cdot [\mathrm{X9}] \tag{25}$$

8.11 Reaction R11

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

Name Phosphorylated bCatenin degradation

Reaction equation

$$\mathrm{X10} \longrightarrow \emptyset \tag{26}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
X10	bCatenin_ast	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k11} \cdot [\mathrm{X10}] \tag{27}$$

8.12 Reaction R12

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

Name bCatenin synthesis

Reaction equation

$$\emptyset \longrightarrow \mathrm{X11} \tag{28}$$

Product

Table 28: Properties of each product.

Id	Name	SBO
X11	bCatenin	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{V12} \tag{29}$$

8.13 Reaction R13

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

Name Unphosphorylated bCatenin degradation

Reaction equation

$$\mathrm{X11} \longrightarrow \emptyset \tag{30}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
X11	bCatenin	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{nucleus}) \cdot \mathrm{k13} \cdot [\mathrm{X11}] \tag{31}$$

8.14 Reaction R14

This is an irreversible reaction of no reactant forming one product influenced by two modifiers.

Name Axin synthesis

Reaction equation

$$\emptyset \xrightarrow{\text{X11, X14}} \text{X12} \tag{32}$$

Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
X11	bCatenin	
X14	bCatenin/TCF	

Product

Table 31: Properties of each product.

Id	Name	SBO
X12	Axin	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol}(\text{nucleus}) \cdot (\text{k14} + \text{k21} \cdot ([\text{X11}] + [\text{X14}])) \tag{33}$$

8.15 Reaction R15

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

Name Axin degradation

Reaction equation

$$\text{X12} \longrightarrow \emptyset \tag{34}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
X12	Axin	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k15} \cdot [\mathrm{X12}] \tag{35}$$

8.16 Reaction R16

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

Name bCatenin/TCF complex formation

Reaction equation

$$\mathrm{X13} + \mathrm{X11} \rightleftharpoons \mathrm{X14} \tag{36}$$

Reactants

Table 33: Properties of each reactant.

Id	Name	SBO
X13	TCF	
X11	bCatenin	

Product

Table 34: Properties of each product.

Id	Name	SBO
X14	bCatenin/TCF	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{nucleus}) \cdot (\mathrm{k\_plus16} \cdot [\mathrm{X11}] \cdot [\mathrm{X13}] - \mathrm{k\_minus16} \cdot [\mathrm{X14}]) \tag{37}$$

8.17 Reaction R17

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

Name APC/bCatenin complex formation

Reaction equation

$$\mathrm{X11} + \mathrm{X7} \rightleftharpoons \mathrm{X15} \tag{38}$$

Reactants

Table 35: Properties of each reactant.

Id	Name	SBO
X11	bCatenin	
X7	APC	

Product

Table 36: Properties of each product.

Id	Name	SBO
X15	bCatenin/APC	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot (\mathrm{k\_plus17} \cdot [\mathrm{X7}] \cdot [\mathrm{X11}] - \mathrm{k\_minus17} \cdot [\mathrm{X15}]) \tag{39}$$

8.18 Reaction R18

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

Name Ras activation

Reaction equation

$$\mathrm{X16} \xrightarrow{\mathrm{X23}} \mathrm{X17} \tag{40}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
X16	Rasi	

Modifier

Table 38: Properties of each modifier.

Id	Name	SBO
X23	ERK_ast	

Product

Table 39: Properties of each product.

Id	Name	SBO
X17	Rasa	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\mathrm{Vmax1} \cdot [\mathrm{X16}] \cdot \mathrm{W}}{\mathrm{Km1} + [\mathrm{X16}]} \cdot \frac{\mathrm{Ki}}{\mathrm{Ki} + [\mathrm{X23}]} \tag{41}$$

8.19 Reaction R19

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

Name Ras inactivation

Reaction equation

$$\mathrm{X17} \longrightarrow \mathrm{X16} \tag{42}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
X17	Rasa	

Product

Table 41: Properties of each product.

Id	Name	SBO
X16	Rasi	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{vol}\,(\text{cytoplasm}) \cdot \frac{\text{Vmax2} \cdot [\text{X17}]}{\text{Km2} + [\text{X17}]} \tag{43}$$

8.20 Reaction R20

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

Name Raf activation

Reaction equation

$$\text{X18} \xrightarrow{\text{X17}} \text{X19} \tag{44}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
X18	Raf-1	

Modifier

Table 43: Properties of each modifier.

Id	Name	SBO
X17	Rasa	

Product

Table 44: Properties of each product.

Id	Name	SBO
X19	Raf-1_ast	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}\,(\text{cytoplasm}) \cdot \frac{\text{kcat1} \cdot [\text{X17}] \cdot [\text{X18}]}{\text{Km3} + [\text{X18}]} \tag{45}$$

8.21 Reaction R21

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

Name Raf inactivation

Reaction equation

$$\text{X19} \longrightarrow \text{X18} \tag{46}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
X19	Raf-1_ast	

Product

Table 46: Properties of each product.

Id	Name	SBO
X18	Raf-1	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \frac{\text{vol}\,(\text{cytoplasm}) \cdot \text{Vmax3} \cdot [\text{X19}]}{\text{Km4} + [\text{X19}]} \tag{47}$$

8.22 Reaction R22

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

Name MEK activation

Reaction equation

$$\mathrm{X20} \xrightarrow{\mathrm{X19}} \mathrm{X21} \tag{48}$$

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
X20	MEK	

Modifier

Table 48: Properties of each modifier.

Id	Name	SBO
X19	Raf-1_ast	

Product

Table 49: Properties of each product.

Id	Name	SBO
X21	MEK_ast	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \frac{\mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{kcat2} \cdot [\mathrm{X19}] \cdot [\mathrm{X20}]}{\mathrm{Km5} + [\mathrm{X20}]} \tag{49}$$

8.23 Reaction R23

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

Name MEK inactivation

Reaction equation

$$\mathrm{X21} \longrightarrow \mathrm{X20} \tag{50}$$

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
X21	MEK_ast	

Product

Table 51: Properties of each product.

Id	Name	SBO
X20	MEK	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \frac{\mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{Vmax4} \cdot [\mathrm{X21}]}{\mathrm{Km6} + [\mathrm{X21}]} \tag{51}$$

8.24 Reaction R24

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

Name ERK activation

Reaction equation

$$\mathrm{X22} \xrightarrow{\mathrm{X21}} \mathrm{X23} \tag{52}$$

Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
X22	ERK	

Modifier

Table 53: Properties of each modifier.

Id	Name	SBO
X21	MEK_ast	

Product

Table 54: Properties of each product.

Id	Name	SBO
X23	ERK_ast	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \frac{\text{vol}\,(\text{cytoplasm}) \cdot \text{kcat3} \cdot [\text{X21}] \cdot [\text{X22}]}{\text{Km7} + [\text{X22}]} \tag{53}$$

8.25 Reaction R25

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

Name ERK inactivation

Reaction equation

$$\text{X23} \longrightarrow \text{X22} \tag{54}$$

Reactant

Table 55: Properties of each reactant.

Id	Name	SBO
X23	ERK_ast	

Product

Table 56: Properties of each product.

Id	Name	SBO
X22	ERK	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \frac{\text{vol}\,(\text{cytoplasm}) \cdot \text{Vmax5} \cdot [\text{X23}]}{\text{Km8} + [\text{X23}]} \tag{55}$$

8.26 Reaction R26

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

Name Raf/RKIP complex disassembly

Reaction equation

$$\text{X24} \xrightarrow{\text{X23}} \text{X18} + \text{X26} \tag{56}$$

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
X24	Raf1/RKIP	

Modifier

Table 58: Properties of each modifier.

Id	Name	SBO
X23	ERK_ast	

Products

Table 59: Properties of each product.

Id	Name	SBO
X18	Raf-1	

Id	Name	SBO
X26	RKIP_ast	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \frac{\text{vol}\,(\text{cytoplasm}) \cdot \text{kcat4} \cdot [\text{X23}] \cdot [\text{X24}]}{\text{Km9} + [\text{X24}]} \tag{57}$$

8.27 Reaction R27

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

Name Raf-RKIP complex formation

Reaction equation

$$\text{X18} + \text{X25} \rightleftharpoons \text{X24} \tag{58}$$

Reactants

Table 60: Properties of each reactant.

Id	Name	SBO
X18	Raf-1	
X25	RKIP	

Product

Table 61: Properties of each product.

Id	Name	SBO
X24	Raf1/RKIP	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \text{vol}\,(\text{cytoplasm}) \cdot (\text{k18} \cdot [\text{X18}] \cdot [\text{X25}] - \text{k19} \cdot [\text{X24}]) \tag{59}$$

8.28 Reaction R28

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

Name RKIP dephosphorylation

Reaction equation

$$\mathrm{X26} \longrightarrow \mathrm{X25} \tag{60}$$

Reactant

Table 62: Properties of each reactant.

Id	Name	SBO
X26	RKIP_ast	

Product

Table 63: Properties of each product.

Id	Name	SBO
X25	RKIP	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \frac{\mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{Vmax6} \cdot [\mathrm{X26}]}{\mathrm{Km10} + [\mathrm{X26}]} \tag{61}$$

8.29 Reaction R29

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

Name Unknown factor-X formation

Reaction equation

$$\emptyset \xrightarrow{\mathrm{X14}} \mathrm{X27} \tag{62}$$

Modifier

Table 64: Properties of each modifier.

Id	Name	SBO
X14	bCatenin/TCF	

Product

Table 65: Properties of each product.

Id	Name	SBO
X27	unknown molecule X	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\mathrm{kcat5} \cdot [\mathrm{X14}]^{\mathrm{n1}}}{\mathrm{Km11}^{\mathrm{n1}} + [\mathrm{X14}]^{\mathrm{n1}}} \tag{63}$$

8.30 Reaction R30

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

Name Factor-X degradation

Reaction equation

$$\mathrm{X27} \longrightarrow \emptyset \tag{64}$$

Reactant

Table 66: Properties of each reactant.

Id	Name	SBO
X27	unknown molecule X	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{k20} \cdot [\mathrm{X27}] \tag{65}$$

8.31 Reaction R31

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

Name Factor-X mediated Raf activation

Reaction equation

$$\mathrm{X18} \xrightarrow{\mathrm{X27}} \mathrm{X19} \tag{66}$$

Reactant

Table 67: Properties of each reactant.

Id	Name	SBO
X18	Raf-1	

Modifier

Table 68: Properties of each modifier.

Id	Name	SBO
X27	unknown molecule X	

Product

Table 69: Properties of each product.

Id	Name	SBO
X19	Raf-1_ast	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\mathrm{kcat6} \cdot [\mathrm{X27}] \cdot [\mathrm{X18}]}{\mathrm{Km12} + [\mathrm{X18}]} \tag{67}$$

8.32 Reaction R32

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

Name ERK mediated GSK3beta phosphorylation

Reaction equation

$$\mathrm{X5} \xrightarrow{\mathrm{X23}} \mathrm{X28} \tag{68}$$

Reactant

Table 70: Properties of each reactant.

Id	Name	SBO
X5	GSK3beta	

Modifier

Table 71: Properties of each modifier.

Id	Name	SBO
X23	ERK_ast	

Product

Table 72: Properties of each product.

Id	Name	SBO
X28	GSK3beta	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \frac{\mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{kcat7} \cdot [\mathrm{X23}] \cdot [\mathrm{X5}]}{\mathrm{Km13} + [\mathrm{X5}]} \tag{69}$$

8.33 Reaction R33

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

Name GSK3beta dephosphorylation

Reaction equation

$$\mathrm{X28} \longrightarrow \mathrm{X5} \tag{70}$$

Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
X28	GSK3beta	

Product

Table 74: Properties of each product.

Id	Name	SBO
X5	GSK3beta	

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \frac{\mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{Vmax7} \cdot [\mathrm{X28}]}{\mathrm{Km14} + [\mathrm{X28}]} \tag{71}$$

9 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.

9.1 Species X1

Name Dshi

Initial concentration $100\ \mathrm{nmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R1 and as a product in R2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X1} = v_2 - v_1 \tag{72}$$

9.2 Species X2

Name Dsha

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

This species takes part in three reactions (as a reactant in R2 and as a product in R1 and as a modifier in R3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X2} = v_1 - v_2 \tag{73}$$

9.3 Species X3

Name APC_ast/Axin_ast/GSK3beta

Initial concentration $0.0153\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in R5, R8 and as a product in R4, R10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X3} = v_4 + v_{10} - v_5 - v_8 \tag{74}$$

9.4 Species X4

Name APC/Axin/GSK3beta

Initial concentration $0.0076\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in R3, R4 and as a product in R5, R6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X4} = v_5 + v_6 - v_3 - v_4 \tag{75}$$

9.5 Species X5

Name GSK3beta

Initial concentration $49.1372\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in R6, R32 and as a product in R3, R33).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X5} = v_3 + v_{33} - v_6 - v_{32} \tag{76}$$

9.6 Species X6

Name APC/Axin

Initial concentration $0.0015\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in R6 and as a product in R3, R7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X6} = v_3 + v_7 - v_6 \tag{77}$$

9.7 Species X7

Name APC

Initial concentration $96.6019\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R7, R17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X7} = -\,v_{7} - v_{17} \tag{78}$$

9.8 Species X8

Name bCatenin/APC_Ast/Axin_ast/GSK3beta

Initial concentration $0.0020\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R9 and as a product in R8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X8} = v_{8} - v_{9} \tag{79}$$

9.9 Species X9

Name bCatenin_ast/APC_ast/Axin_ast/GSK3beta

Initial concentration $0.0020\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R10 and as a product in R9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X9} = v_{9} - v_{10} \tag{80}$$

9.10 Species X10

Name bCatenin_ast

Initial concentration $0.9881\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R11 and as a product in R10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X10} = v_{10} - v_{11} \tag{81}$$

9.11 Species X11

Name bCatenin

Initial concentration $42.7224\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in R8, R13, R16, R17 and as a product in R12 and as a modifier in R14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X11} = v_{12} - v_{8} - v_{13} - v_{16} - v_{17} \tag{82}$$

9.12 Species X12

Name Axin

Initial concentration $8 \cdot 10^{-4}$ nmol $\cdot$ l^{-1}

This species takes part in three reactions (as a reactant in R7, R15 and as a product in R14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X12} = v_{14} - v_{7} - v_{15} \tag{83}$$

9.13 Species X13

Name TCF

Initial concentration 6.1879 nmol $\cdot$ l^{-1}

This species takes part in one reaction (as a reactant in R16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X13} = -v_{16} \tag{84}$$

9.14 Species X14

Name bCatenin/TCF

Initial concentration 8.8121 nmol $\cdot$ l^{-1}

This species takes part in three reactions (as a product in R16 and as a modifier in R14, R29).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X14} = v_{16} \tag{85}$$

9.15 Species X15

Name bCatenin/APC

Initial concentration 3.4392 nmol $\cdot$ l^{-1}

This species takes part in one reaction (as a product in R17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X15} = v_{17} \tag{86}$$

9.16 Species X16

Name Rasi

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

This species takes part in two reactions (as a reactant in R18 and as a product in R19).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X16} = v_{19} - v_{18} \tag{87}$$

9.17 Species X17

Name Rasa

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

This species takes part in three reactions (as a reactant in R19 and as a product in R18 and as a modifier in R20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X17} = v_{18} - v_{19} \tag{88}$$

9.18 Species X18

Name Raf-1

Initial concentration $112.5585\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in R20, R27, R31 and as a product in R21, R26).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X18} = v_{21} + v_{26} - v_{20} - v_{27} - v_{31} \tag{89}$$

9.19 Species X19

Name Raf-1_ast

Initial concentration $6.486\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in R21 and as a product in R20, R31 and as a modifier in R22).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X19} = v_{20} + v_{31} - v_{21} \tag{90}$$

9.20 Species X20

Name MEK

Initial concentration $296.1137\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R22 and as a product in R23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X20} = v_{23} - v_{22} \tag{91}$$

9.21 Species X21

Name MEK_ast

Initial concentration 3.8863 nmol · l^{-1}

This species takes part in three reactions (as a reactant in R23 and as a product in R22 and as a modifier in R24).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X21} = v_{22} - v_{23} \tag{92}$$

9.22 Species X22

Name ERK

Initial concentration 297.8897 nmol · l^{-1}

This species takes part in two reactions (as a reactant in R24 and as a product in R25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X22} = v_{25} - v_{24} \tag{93}$$

9.23 Species X23

Name ERK_ast

Initial concentration 2.1103 nmol · l^{-1}

This species takes part in five reactions (as a reactant in R25 and as a product in R24 and as a modifier in R18, R26, R32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X23} = v_{24} - v_{25} \tag{94}$$

9.24 Species X24

Name Raf1/RKIP

Initial concentration 180.9595 nmol · l^{-1}

This species takes part in two reactions (as a reactant in R26 and as a product in R27).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X24} = v_{27} - v_{26} \tag{95}$$

9.25 Species X25

Name RKIP

Initial concentration $418.1788\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R27 and as a product in R28).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X25} = v_{28} - v_{27} \tag{96}$$

9.26 Species X26

Name RKIP_ast

Initial concentration $0.8619\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R28 and as a product in R26).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X26} = v_{26} - v_{28} \tag{97}$$

9.27 Species X27

Name unknown molecule X

Initial concentration $10.263\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in R30 and as a product in R29 and as a modifier in R31).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X27} = v_{29} - v_{30} \tag{98}$$

9.28 Species X28

Name GSK3beta

Initial concentration $0.85544\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R33 and as a product in R32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X28} = v_{32} - v_{33} \tag{99}$$

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