

SBML Model Report

**Model name: “Hockin1999-
_BloodCoagulation_Valnactivation”**



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Michael Schubert¹ at August 26th 2011 at 4:38 p. m. and last time modified at October ninth 2014 at 5:17 p. m. Table 1 shows an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	30
events	0	constraints	0
reactions	33	function definitions	0
global parameters	9	unit definitions	0
rules	0	initial assignments	0

2 Unit Definitions

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

¹EBI, schubert@ebi.ac.uk

2.1 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

2.2 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.3 Unit area

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

Definition m²

2.4 Unit length

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

Definition m

2.5 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment_1	compartment_1		3	1	litre	<input checked="" type="checkbox"/>	

3.1 Compartment compartment_1

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

Name compartment_1

4 Species

This model contains 30 species. Section 7 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
APC	APC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va	Va	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va_APC	Va_APC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va3	Va3	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va3_APC	Va3_APC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va5	Va5	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va5_APC	Va5_APC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va53	Va53	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va53_APC	Va53_APC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va56	Va56	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va56_APC	Va56_APC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va36	Va36	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va36_APC	Va36_APC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va536	Va536	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
Va536_APC	Va536_APC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
HC	HC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
LC	LC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
HC5	HC5	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
HC3	HC3	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
HC56	HC56	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
HC36	HC36	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square
HC536	HC536	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	\square	\square

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
LC_APC	LC_APC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
HC53	HC53	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
VaA3	VaA3	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
VaA53	VaA53	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
VaA36	VaA36	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
VaA536	VaA536	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
VaLCA1	VaLCA1	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
VaLCA1_APC	VaLCA1_APC	compartment_1	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>

5 Parameters

This model contains nine global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000036	10^8		✓
k2	k2	0000038	0.700		✓
k3	k3	0000035	0.064		✓
k5	k5	0000035	1.000		✓
k6	k6	0000035	$5.2 \cdot 10^{-4}$		✓
k7	k7	0000035	0.028		✓
k8	k8	0000039	2570.000		✓
k9	k9	0000035	$1.72 \cdot 10^{-5}$		✓
k10	k10	0000039	2630.000		✓

6 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

Nº	Id	Name	Reaction Equation	SBO
1	r1	r1	$Va + APC \rightleftharpoons Va_APC$	
2	r2	r2	$Va3 + APC \rightleftharpoons Va3_APC$	
3	r3	r3	$Va5 + APC \rightleftharpoons Va5_APC$	
4	r4	r4	$Va53 + APC \rightleftharpoons Va53_APC$	
5	r5	r5	$Va56 + APC \rightleftharpoons Va56_APC$	
6	r6	r6	$Va36 + APC \rightleftharpoons Va36_APC$	
7	r7	r7	$Va536 + APC \rightleftharpoons Va536_APC$	
8	r8	r8	$Va_APC \longrightarrow Va5_APC$	
9	r9	r9	$Va5_APC \longrightarrow Va56_APC$	
10	r10	r10	$Va56_APC \longrightarrow Va536_APC$	
11	r11	r11	$Va5_APC \longrightarrow Va53_APC$	
12	r12	r12	$Va53_APC \longrightarrow Va536_APC$	
13	r13	r13	$Va_APC \longrightarrow Va3_APC$	
14	r14	r14	$Va3_APC \longrightarrow Va36_APC$	
15	r15	r15	$Va36_APC \longrightarrow Va536_APC$	
16	r16	r16	$Va3_APC \longrightarrow Va53_APC$	
17	r17	r17	$Va \rightleftharpoons HC + LC$	
18	r18	r18	$Va5 \rightleftharpoons HC5 + LC$	
19	r19	r19	$Va3 \rightleftharpoons HC3 + LC$	
20	r20	r20	$Va56 \rightleftharpoons HC56 + LC$	
21	r21	r21	$Va53 \rightleftharpoons HC53 + LC$	
22	r22	r22	$Va36 \rightleftharpoons HC36 + LC$	
23	r23	r23	$Va536 \rightleftharpoons HC536 + LC$	

Nº	Id	Name	Reaction Equation	SBO
24	r24	r24	$LC + APC \rightleftharpoons LC_APC$	
25	r25	r25	$Va3 \rightleftharpoons VaA3 + VaLCA1$	
26	r26	r26	$Va53 \rightleftharpoons VaA53 + VaLCA1$	
27	r27	r27	$Va36 \rightleftharpoons VaA36 + VaLCA1$	
28	r28	r28	$Va536 \rightleftharpoons VaA536 + VaLCA1$	
29	r29	r29	$Va3_APC \rightleftharpoons VaA3 + VaLCA1_APC$	
30	r30	r30	$Va53_APC \rightleftharpoons VaA53 + VaLCA1_APC$	
31	r31	r31	$Va36_APC \rightleftharpoons VaA36 + VaLCA1_APC$	
32	r32	r32	$Va536_APC \rightleftharpoons VaA536 + VaLCA1_APC$	
33	r33	r33	$VaLCA1 + APC \rightleftharpoons VaLCA1_APC$	

6.1 Reaction r1

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

Name r1

Reaction equation



Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
Va	Va	0000010
APC	APC	0000010

Product

Table 7: Properties of each product.

Id	Name	SBO
Va_APC	Va_APC	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{compartment}_1) \cdot (k_1 \cdot [\text{Va}] \cdot [\text{APC}] - k_2 \cdot [\text{Va_APC}]) \quad (2)$$

6.2 Reaction r2

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

Name r2

Reaction equation



Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
Va3	Va3	0000010
APC	APC	0000010

Product

Table 9: Properties of each product.

Id	Name	SBO
Va3_APC	Va3_APC	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_2 = \text{vol}(\text{compartment}_1) \cdot (k_1 \cdot [\text{Va3}] \cdot [\text{APC}] - k_2 \cdot [\text{Va3_APC}]) \quad (4)$$

6.3 Reaction r3

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

Name r3

Reaction equation



Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
Va5	Va5	0000010
APC	APC	0000010

Product

Table 11: Properties of each product.

Id	Name	SBO
Va5_APC	Va5_APC	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{compartment}_1) \cdot (k_1 \cdot [\text{Va5}] \cdot [\text{APC}] - k_2 \cdot [\text{Va5_APC}]) \quad (6)$$

6.4 Reaction r4

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

Name r4

Reaction equation



Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
Va53	Va53	0000010
APC	APC	0000010

Product

Table 13: Properties of each product.

Id	Name	SBO
Va53_APC	Va53_APC	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_4 = \text{vol}(\text{compartment}_1) \cdot (k_1 \cdot [\text{Va53}] \cdot [\text{APC}] - k_2 \cdot [\text{Va53_APC}]) \quad (8)$$

6.5 Reaction r5

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

Name r5

Reaction equation



Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
Va56	Va56	0000010
APC	APC	0000010

Product

Table 15: Properties of each product.

Id	Name	SBO
Va56_APC	Va56_APC	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_5 = \text{vol}(\text{compartment}_1) \cdot (k_1 \cdot [\text{Va56}] \cdot [\text{APC}] - k_2 \cdot [\text{Va56_APC}]) \quad (10)$$

6.6 Reaction r6

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

Name r6

Reaction equation



Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
Va36	Va36	0000010
APC	APC	0000010

Product

Table 17: Properties of each product.

Id	Name	SBO
Va36_APC	Va36_APC	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_6 = \text{vol}(\text{compartment_1}) \cdot (k_1 \cdot [\text{Va36}] \cdot [\text{APC}] - k_2 \cdot [\text{Va36_APC}]) \quad (12)$$

6.7 Reaction r7

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

Name r7

Reaction equation



Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
Va536	Va536	0000010
APC	APC	0000010

Product

Table 19: Properties of each product.

Id	Name	SBO
Va536_APC	Va536_APC	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_7 = \text{vol}(\text{compartment}_1) \cdot (k_1 \cdot [\text{Va536}] \cdot [\text{APC}] - k_2 \cdot [\text{Va536_APC}]) \quad (14)$$

6.8 Reaction r8

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

Name r8

Reaction equation



Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
Va_APC	Va_APC	0000010

Product

Table 21: Properties of each product.

Id	Name	SBO
Va5_APC	Va5_APC	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_8 = \text{vol}(\text{compartment}_1) \cdot k_5 \cdot [\text{Va_APC}] \quad (16)$$

6.9 Reaction r9

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

Name r9

Reaction equation



Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
Va5_APC	Va5_APC	0000010

Product

Table 23: Properties of each product.

Id	Name	SBO
Va56_APC	Va56_APC	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_9 = \text{vol}(\text{compartment}_1) \cdot k_6 \cdot [\text{Va5_APC}] \quad (18)$$

6.10 Reaction r10

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

Name r10

Reaction equation



Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
Va56_APC	Va56_APC	0000010

Product

Table 25: Properties of each product.

Id	Name	SBO
Va536_APC	Va536_APC	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_{10} = \text{vol}(\text{compartment_1}) \cdot k_3 \cdot [\text{Va56_APC}] \quad (20)$$

6.11 Reaction r11

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

Name r11

Reaction equation



Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
Va5_APC	Va5_APC	0000010

Product

Table 27: Properties of each product.

Id	Name	SBO
Va53_APC	Va53_APC	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_{11} = \text{vol}(\text{compartment_1}) \cdot k_3 \cdot [\text{Va5_APC}] \quad (22)$$

6.12 Reaction r12

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

Name r12

Reaction equation



Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
Va53_APC	Va53_APC	0000010

Product

Table 29: Properties of each product.

Id	Name	SBO
Va536_APC	Va536_APC	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_{12} = \text{vol}(\text{compartment}_1) \cdot k_6 \cdot [\text{Va53_APC}] \quad (24)$$

6.13 Reaction r13

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

Name r13

Reaction equation



Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
Va_APC	Va_APC	0000010

Product

Table 31: Properties of each product.

Id	Name	SBO
Va3_APC	Va3_APC	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_{13} = \text{vol}(\text{compartment}_1) \cdot k_3 \cdot [\text{Va_APC}] \quad (26)$$

6.14 Reaction r14

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

Name r14

Reaction equation



Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
Va3_APC	Va3_APC	0000010

Product

Table 33: Properties of each product.

Id	Name	SBO
Va36_APC	Va36_APC	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_{14} = \text{vol}(\text{compartment_1}) \cdot k_6 \cdot [\text{Va3_APC}] \quad (28)$$

6.15 Reaction r15

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

Name r15

Reaction equation



Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
Va36_APC	Va36_APC	0000010

Product

Table 35: Properties of each product.

Id	Name	SBO
Va536_APC	Va536_APC	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_{15} = \text{vol}(\text{compartment}_1) \cdot k_5 \cdot [\text{Va36_APC}] \quad (30)$$

6.16 Reaction r16

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

Name r16

Reaction equation



Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
Va3_APC	Va3_APC	0000010

Product

Table 37: Properties of each product.

Id	Name	SBO
Va53_APC	Va53_APC	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_{16} = \text{vol}(\text{compartment}_1) \cdot k_5 \cdot [\text{Va3_APC}] \quad (32)$$

6.17 Reaction r17

This is a reversible reaction of one reactant forming two products.

Name r17

Reaction equation



Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
Va	Va	0000010

Products

Table 39: Properties of each product.

Id	Name	SBO
HC	HC	0000011
LC	LC	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

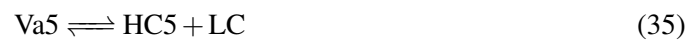
$$v_{17} = \text{vol}(\text{compartment_1}) \cdot (k_9 \cdot [\text{Va}] - k_{10} \cdot [\text{HC}] \cdot [\text{LC}]) \quad (34)$$

6.18 Reaction r18

This is a reversible reaction of one reactant forming two products.

Name r18

Reaction equation



Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
Va5	Va5	0000010

Products

Table 41: Properties of each product.

Id	Name	SBO
HC5	HC5	0000011
LC	LC	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{18} = \text{vol}(\text{compartment_1}) \cdot (k_9 \cdot [\text{Va5}] - k_{10} \cdot [\text{HC5}] \cdot [\text{LC}]) \quad (36)$$

6.19 Reaction r19

This is a reversible reaction of one reactant forming two products.

Name r19

Reaction equation



Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
Va3	Va3	0000010

Products

Table 43: Properties of each product.

Id	Name	SBO
HC3	HC3	0000011
LC	LC	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{19} = \text{vol}(\text{compartment_1}) \cdot (k_9 \cdot [\text{Va3}] - k_{10} \cdot [\text{HC3}] \cdot [\text{LC}]) \quad (38)$$

6.20 Reaction r20

This is a reversible reaction of one reactant forming two products.

Name r20

Reaction equation



Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
Va56	Va56	0000010

Products

Table 45: Properties of each product.

Id	Name	SBO
HC56	HC56	0000011
LC	LC	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{20} = \text{vol}(\text{compartment}_1) \cdot (k_9 \cdot [\text{Va56}] - k_{10} \cdot [\text{HC56}] \cdot [\text{LC}]) \quad (40)$$

6.21 Reaction r21

This is a reversible reaction of one reactant forming two products.

Name r21

Reaction equation



Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
Va53	Va53	0000010

Products

Table 47: Properties of each product.

Id	Name	SBO
HC53	HC53	0000011
LC	LC	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

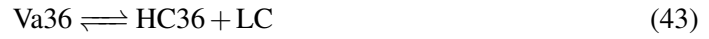
$$v_{21} = \text{vol}(\text{compartment}_1) \cdot (k_9 \cdot [\text{Va53}] - k_{10} \cdot [\text{HC53}] \cdot [\text{LC}]) \quad (42)$$

6.22 Reaction r22

This is a reversible reaction of one reactant forming two products.

Name r22

Reaction equation



Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
Va36	Va36	0000010

Products

Table 49: Properties of each product.

Id	Name	SBO
HC36	HC36	0000011
LC	LC	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{22} = \text{vol}(\text{compartment_1}) \cdot (k_9 \cdot [\text{Va36}] - k_{10} \cdot [\text{HC36}] \cdot [\text{LC}]) \quad (44)$$

6.23 Reaction r23

This is a reversible reaction of one reactant forming two products.

Name r23

Reaction equation



Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
Va536	Va536	0000010

Products

Table 51: Properties of each product.

Id	Name	SBO
HC536	HC536	0000011
LC	LC	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{23} = \text{vol}(\text{compartment_1}) \cdot (k_9 \cdot [\text{Va536}] - k_{10} \cdot [\text{HC536}] \cdot [\text{LC}]) \quad (46)$$

6.24 Reaction r24

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

Name r24

Reaction equation



Reactants

Table 52: Properties of each reactant.

Id	Name	SBO
LC	LC	0000010
APC	APC	0000010

Product

Table 53: Properties of each product.

Id	Name	SBO
LC_APC	LC_APC	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_{24} = \text{vol}(\text{compartment}_1) \cdot (k_1 \cdot [\text{LC}] \cdot [\text{APC}] - k_2 \cdot [\text{LC_APC}]) \quad (48)$$

6.25 Reaction r25

This is a reversible reaction of one reactant forming two products.

Name r25

Reaction equation



Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
Va3	Va3	0000010

Products

Table 55: Properties of each product.

Id	Name	SBO
VaA3	VaA3	0000011
VaLCA1	VaLCA1	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{25} = \text{vol}(\text{compartment_1}) \cdot (k7 \cdot [\text{Va3}] - k8 \cdot [\text{VaA3}] \cdot [\text{VaLCA1}]) \quad (50)$$

6.26 Reaction r26

This is a reversible reaction of one reactant forming two products.

Name r26

Reaction equation



Reactant

Table 56: Properties of each reactant.

Id	Name	SBO
Va53	Va53	0000010

Products

Table 57: Properties of each product.

Id	Name	SBO
VaA53	VaA53	0000011
VaLCA1	VaLCA1	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{26} = \text{vol}(\text{compartment}_1) \cdot (k_7 \cdot [\text{Va53}] - k_8 \cdot [\text{VaA53}] \cdot [\text{VaLCA1}]) \quad (52)$$

6.27 Reaction r27

This is a reversible reaction of one reactant forming two products.

Name r27

Reaction equation



Reactant

Table 58: Properties of each reactant.

Id	Name	SBO
Va36	Va36	0000010

Products

Table 59: Properties of each product.

Id	Name	SBO
VaA36	VaA36	0000011
VaLCA1	VaLCA1	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{27} = \text{vol}(\text{compartment_1}) \cdot (k7 \cdot [\text{Va36}] - k8 \cdot [\text{VaA36}] \cdot [\text{VaLCA1}]) \quad (54)$$

6.28 Reaction r28

This is a reversible reaction of one reactant forming two products.

Name r28

Reaction equation



Reactant

Table 60: Properties of each reactant.

Id	Name	SBO
Va536	Va536	0000010

Products

Table 61: Properties of each product.

Id	Name	SBO
VaA536	VaA536	0000011
VaLCA1	VaLCA1	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{28} = \text{vol}(\text{compartment_1}) \cdot (k7 \cdot [\text{Va536}] - k8 \cdot [\text{VaA536}] \cdot [\text{VaLCA1}]) \quad (56)$$

6.29 Reaction r29

This is a reversible reaction of one reactant forming two products.

Name r29

Reaction equation



Reactant

Table 62: Properties of each reactant.

Id	Name	SBO
Va3_APC	Va3_APC	0000010

Products

Table 63: Properties of each product.

Id	Name	SBO
VaA3	VaA3	0000011
VaLCA1_APC	VaLCA1_APC	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{29} = \text{vol}(\text{compartment}_1) \cdot (k7 \cdot [\text{Va3_APC}] - k8 \cdot [\text{VaA3}] \cdot [\text{VaLCA1_APC}]) \quad (58)$$

6.30 Reaction r30

This is a reversible reaction of one reactant forming two products.

Name r30

Reaction equation



Reactant

Table 64: Properties of each reactant.

Id	Name	SBO
Va53_APC	Va53_APC	0000010

Products

Table 65: Properties of each product.

Id	Name	SBO
VaA53	VaA53	0000011
VaLCA1_APC	VaLCA1_APC	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{30} = \text{vol}(\text{compartment}_1) \cdot (k_7 \cdot [\text{Va53_APC}] - k_8 \cdot [\text{VaA53}] \cdot [\text{VaLCA1_APC}]) \quad (60)$$

6.31 Reaction r31

This is a reversible reaction of one reactant forming two products.

Name r31

Reaction equation



Reactant

Table 66: Properties of each reactant.

Id	Name	SBO
Va36_APC	Va36_APC	0000010

Products

Table 67: Properties of each product.

Id	Name	SBO
VaA36	VaA36	0000011
VaLCA1_APC	VaLCA1_APC	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_{31} = \text{vol}(\text{compartment}_1) \cdot (k_7 \cdot [\text{Va36_APC}] - k_8 \cdot [\text{VaA36}] \cdot [\text{VaLCA1_APC}]) \quad (62)$$

6.32 Reaction r32

This is a reversible reaction of one reactant forming two products.

Name r32

Reaction equation



Reactant

Table 68: Properties of each reactant.

Id	Name	SBO
Va536_APC	Va536_APC	0000010

Products

Table 69: Properties of each product.

Id	Name	SBO
VaA536	VaA536	0000011
VaLCA1_APC	VaLCA1_APC	0000011

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \text{vol}(\text{compartment}_1) \cdot (k7 \cdot [\text{Va536_APC}] - k7 \cdot [\text{VaA536}] \cdot [\text{VaLCA1_APC}]) \quad (64)$$

6.33 Reaction r33

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

Name r33

Reaction equation



Reactants

Table 70: Properties of each reactant.

Id	Name	SBO
VaLCA1	VaLCA1	0000010
APC	APC	0000010

Product

Table 71: Properties of each product.

Id	Name	SBO
VaLCA1_APC	VaLCA1_APC	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_{33} = \text{vol}(\text{compartment}_1) \cdot (k1 \cdot [\text{VaLCA1}] \cdot [\text{APC}] - k2 \cdot [\text{VaLCA1_APC}]) \quad (66)$$

7 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML substance per time. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or
- volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions > 0` for certain species.

7.1 Species APC

Name APC

Initial concentration $10^{-8} \text{ mol} \cdot \text{l}^{-1}$

This species takes part in nine reactions (as a reactant in [r1](#), [r2](#), [r3](#), [r4](#), [r5](#), [r6](#), [r7](#), [r24](#), [r33](#)).

$$\frac{d}{dt} \text{APC} = -v_1 - v_2 - v_3 - v_4 - v_5 - v_6 - v_7 - v_{24} - v_{33} \quad (67)$$

7.2 Species Va

Name Va

Initial concentration $2 \cdot 10^{-7} \text{ mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [r1](#), [r17](#)).

$$\frac{d}{dt} \text{Va} = -v_1 - v_{17} \quad (68)$$

7.3 Species Va_APC

Name Va_APC

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

This species takes part in three reactions (as a reactant in [r8](#), [r13](#) and as a product in [r1](#)).

$$\frac{d}{dt} \text{Va_APC} = v_1 - v_8 - v_{13} \quad (69)$$

7.4 Species Va3

Name Va3

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

This species takes part in three reactions (as a reactant in [r2](#), [r19](#), [r25](#)).

$$\frac{d}{dt} \text{Va3} = -v_2 - v_{19} - v_{25} \quad (70)$$

7.5 Species Va3_APC

Name Va3_APC

Initial concentration 0 mol · l⁻¹

This species takes part in five reactions (as a reactant in r14, r16, r29 and as a product in r2, r13).

$$\frac{d}{dt} \text{Va3_APC} = v_2 + v_{13} - v_{14} - v_{16} - v_{29} \quad (71)$$

7.6 Species Va5

Name Va5

Initial concentration 0 mol · l⁻¹

This species takes part in two reactions (as a reactant in r3, r18).

$$\frac{d}{dt} \text{Va5} = -v_3 - v_{18} \quad (72)$$

7.7 Species Va5_APC

Name Va5_APC

Initial concentration 0 mol · l⁻¹

This species takes part in four reactions (as a reactant in r9, r11 and as a product in r3, r8).

$$\frac{d}{dt} \text{Va5_APC} = v_3 + v_8 - v_9 - v_{11} \quad (73)$$

7.8 Species Va53

Name Va53

Initial concentration 0 mol · l⁻¹

This species takes part in three reactions (as a reactant in r4, r21, r26).

$$\frac{d}{dt} \text{Va53} = -v_4 - v_{21} - v_{26} \quad (74)$$

7.9 Species Va53_APC

Name Va53_APC

Initial concentration 0 mol · l⁻¹

This species takes part in five reactions (as a reactant in [r12](#), [r30](#) and as a product in [r4](#), [r11](#), [r16](#)).

$$\frac{d}{dt} \text{Va53_APC} = v_4 + v_{11} + v_{16} - v_{12} - v_{30} \quad (75)$$

7.10 Species Va56

Name Va56

Initial concentration 0 mol · l⁻¹

This species takes part in two reactions (as a reactant in [r5](#), [r20](#)).

$$\frac{d}{dt} \text{Va56} = -v_5 - v_{20} \quad (76)$$

7.11 Species Va56_APC

Name Va56_APC

Initial concentration 0 mol · l⁻¹

This species takes part in three reactions (as a reactant in [r10](#) and as a product in [r5](#), [r9](#)).

$$\frac{d}{dt} \text{Va56_APC} = v_5 + v_9 - v_{10} \quad (77)$$

7.12 Species Va36

Name Va36

Initial concentration 0 mol · l⁻¹

This species takes part in three reactions (as a reactant in [r6](#), [r22](#), [r27](#)).

$$\frac{d}{dt} \text{Va36} = -v_6 - v_{22} - v_{27} \quad (78)$$

7.13 Species Va36_APC

Name Va36_APC

Initial concentration 0 mol · l⁻¹

This species takes part in four reactions (as a reactant in [r15](#), [r31](#) and as a product in [r6](#), [r14](#)).

$$\frac{d}{dt} \text{Va36_APC} = v_6 + v_{14} - v_{15} - v_{31} \quad (79)$$

7.14 Species Va536

Name Va536

Initial concentration 0 mol · l⁻¹

This species takes part in three reactions (as a reactant in [r7](#), [r23](#), [r28](#)).

$$\frac{d}{dt}\text{Va536} = -v_7 - v_{23} - v_{28} \quad (80)$$

7.15 Species Va536_APC

Name Va536_APC

Initial concentration 0 mol · l⁻¹

This species takes part in five reactions (as a reactant in [r32](#) and as a product in [r7](#), [r10](#), [r12](#), [r15](#)).

$$\frac{d}{dt}\text{Va536_APC} = v_7 + v_{10} + v_{12} + v_{15} - v_{32} \quad (81)$$

7.16 Species HC

Name HC

Initial concentration 0 mol · l⁻¹

This species takes part in one reaction (as a product in [r17](#)).

$$\frac{d}{dt}\text{HC} = v_{17} \quad (82)$$

7.17 Species LC

Name LC

Initial concentration 0 mol · l⁻¹

This species takes part in eight reactions (as a reactant in [r24](#) and as a product in [r17](#), [r18](#), [r19](#), [r20](#), [r21](#), [r22](#), [r23](#)).

$$\frac{d}{dt}\text{LC} = v_{17} + v_{18} + v_{19} + v_{20} + v_{21} + v_{22} + v_{23} - v_{24} \quad (83)$$

7.18 Species HC5

Name HC5

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

This species takes part in one reaction (as a product in [r18](#)).

$$\frac{d}{dt}\text{HC5} = v_{18} \quad (84)$$

7.19 Species HC3

Name HC3

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

This species takes part in one reaction (as a product in [r19](#)).

$$\frac{d}{dt}\text{HC3} = v_{19} \quad (85)$$

7.20 Species HC56

Name HC56

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

This species takes part in one reaction (as a product in [r20](#)).

$$\frac{d}{dt}\text{HC56} = v_{20} \quad (86)$$

7.21 Species HC36

Name HC36

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

This species takes part in one reaction (as a product in [r22](#)).

$$\frac{d}{dt}\text{HC36} = v_{22} \quad (87)$$

7.22 Species HC536

Name HC536

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

This species takes part in one reaction (as a product in [r23](#)).

$$\frac{d}{dt}\text{HC536} = v_{23} \quad (88)$$

7.23 Species LC_APC

Name LC_APC

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

This species takes part in one reaction (as a product in [r24](#)).

$$\frac{d}{dt} \text{LC_APC} = v_{24} \quad (89)$$

7.24 Species HC53

Name HC53

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

This species takes part in one reaction (as a product in [r21](#)).

$$\frac{d}{dt} \text{HC53} = v_{21} \quad (90)$$

7.25 Species VaA3

Name VaA3

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

This species takes part in two reactions (as a product in [r25](#), [r29](#)).

$$\frac{d}{dt} \text{VaA3} = v_{25} + v_{29} \quad (91)$$

7.26 Species VaA53

Name VaA53

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

This species takes part in two reactions (as a product in [r26](#), [r30](#)).

$$\frac{d}{dt} \text{VaA53} = v_{26} + v_{30} \quad (92)$$

7.27 Species VaA36

Name VaA36

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

This species takes part in two reactions (as a product in [r27](#), [r31](#)).

$$\frac{d}{dt} \text{VaA36} = v_{27} + v_{31} \quad (93)$$

7.28 Species VaA536

Name VaA536

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

This species takes part in two reactions (as a product in [r28](#), [r32](#)).

$$\frac{d}{dt} \text{VaA536} = v_{28} + v_{32} \quad (94)$$

7.29 Species VaLCA1

Name VaLCA1

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

This species takes part in five reactions (as a reactant in [r33](#) and as a product in [r25](#), [r26](#), [r27](#), [r28](#)).

$$\frac{d}{dt} \text{VaLCA1} = v_{25} + v_{26} + v_{27} + v_{28} - v_{33} \quad (95)$$

7.30 Species VaLCA1_APC

Name VaLCA1_APC

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

This species takes part in five reactions (as a product in [r29](#), [r30](#), [r31](#), [r32](#), [r33](#)).

$$\frac{d}{dt} \text{VaLCA1_APC} = v_{29} + v_{30} + v_{31} + v_{32} + v_{33} \quad (96)$$

A Glossary of Systems Biology Ontology Terms

SBO:0000010 reactant: Substance consumed by a chemical reaction. Reactants react with each other to form the products of a chemical reaction. In a chemical equation the Reactants are the elements or compounds on the left hand side of the reaction equation. A reactant can be consumed and produced by the same reaction, its global quantity remaining unchanged

SBO:0000011 product: Substance that is produced in a reaction. In a chemical equation the Products are the elements or compounds on the right hand side of the reaction equation. A product can be produced and consumed by the same reaction, its global quantity remaining unchanged

SBO:0000035 forward unimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving only one reactant. This parameter encompasses all the contributions to the velocity except the quantity of the reactant. It is to be used in a reaction modelled using a continuous framework

SBO:0000036 forward bimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving two reactants. This parameter encompasses all the contributions to the velocity except the quantity of the reactants. It is to be used in a reaction modelled using a continuous framework

SBO:0000038 reverse unimolecular rate constant, continuous case: Numerical parameter that quantifies the reverse velocity of a chemical reaction involving only one product. This parameter encompasses all the contributions to the velocity except the quantity of the product. It is to be used in a reaction modelled using a continuous framework

SBO:0000039 reverse bimolecular rate constant, continuous case: Numerical parameter that quantifies the reverse velocity of a chemical reaction involving only one product. This parameter encompasses all the contributions to the velocity except the quantity of the product. It is to be used in a reaction modelled using a continuous framework

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does not include any reverse process that creates the reactants from the products. The change of a product quantity is proportional to the quantity of one reactant. It is to be used in a reaction modelled using a continuous framework.

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does include a reverse process that creates the reactants from the products. The rate of the forward process is proportional to the quantity of one reactant. The rate of the reverse process is proportional to the product of two product quantities. It is to be used in a reaction modelled using a continuous framework.

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does include a reverse process that creates the reactants from the products. The rate of the forward process is proportional to the product of two reactant quantities. The rate of the reverse process is proportional to the quantity of one product. It is to be used in a reaction modelled using a continuous framework.

SBML²TeX was developed by Andreas Dräger^a, Hannes Planatscher^a, Dieudonné M Wouamba^a, Adrian Schröder^a, Michael Hucka^b, Lukas Endler^c, Martin Golebiewski^d and Andreas Zell^a. Please see <http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX> for more information.

^aCenter for Bioinformatics Tübingen (ZBIT), Germany

^bCalifornia Institute of Technology, Beckman Institute BNMC, Pasadena, United States

^cEuropean Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom

^dEML Research gGmbH, Heidelberg, Germany