

SBML Model Report

Model name:
“Lee2010_ThrombinActivation_OneForm”



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 4:37 p. m. and last time modified at May 28th 2014 at 4:38 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	14
events	0	constraints	0
reactions	16	function definitions	0
global parameters	22	unit definitions	1
rules	0	initial assignments	0

2 Unit Definitions

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

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2.1 Unit substance

Name substance

Definition μmol

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 m^2

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	compartment		3	1	litre	<input checked="" type="checkbox"/>	

3.1 Compartment compartment

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

Name compartment

4 Species

This model contains 14 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
E	E	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
E_P_1	E_P_1	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
P	P	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
M	M	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
M1	M1	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
E_M1	E_M1	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
E_M	E_M	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
T	T	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
E_P_2	E_P_2	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
P2	P2	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
P21	P21	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
E_P21	E_P21	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
E_P2	E_P2	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
E_P1	E_P1	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square

5 Parameters

This model contains 22 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000036	91.800		✓
k2	k2	0000035	82.400		✓
k9	k9	0000035	$3.12 \cdot 10^{-8}$		✓
k3	k3	0000036	38.100		✓
k3a	k3a	0000036	151.500		✓
k4	k4	0000035	38.100		✓
k4a	k4a	0000035	209.900		✓
k5	k5	0000036	5.160		✓
k6	k6	0000035	32.300		✓
k10	k10	0000035	$7.23 \cdot 10^{-10}$		✓
k7	k7	0000036	$6.76 \cdot 10^{-8}$		✓
k7a	k7a	0000036	4.700		✓
k8	k8	0000035	0.006		✓
k8a	k8a	0000035	42.600		✓
kC1	kC1	0000035	$2.39 \cdot 10^{-6}$		✓
kC2	kC2	0000035	0.031		✓
j1	j1	0000038	33.400		✓
j3	j3	0000038	$1.58 \cdot 10^{-6}$		✓
j3a	j3a	0000038	0.185		✓
j5	j5	0000038	21.800		✓
j7	j7	0000038	$4.46 \cdot 10^{-9}$		✓
j7a	j7a	0000038	$2.66 \cdot 10^{-5}$		✓

6 Reactions

This model contains 16 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	$E + P \rightleftharpoons E_P_1$	
2	r2	r2	$E_P_1 \longrightarrow E + M$	
3	r3	r3	$M \longrightarrow M1$	
4	r4	r4	$E + M1 \rightleftharpoons E_M1$	
5	r5	r5	$E + M \rightleftharpoons E_M$	
6	r6	r6	$E_M1 \longrightarrow E + T$	
7	r7	r7	$E_M \longrightarrow E + T$	
8	r8	r8	$E + P \rightleftharpoons E_P_2$	
9	r9	r9	$E_P_2 \longrightarrow E + P2$	
10	r10	r10	$P2 \longrightarrow P21$	
11	r11	r11	$E + P21 \rightleftharpoons E_P21$	
12	r12	r12	$E + P2 \rightleftharpoons E_P2$	
13	r13	r13	$E_P21 \longrightarrow E + T$	
14	r14	r14	$E_P2 \longrightarrow E + T$	
15	r15	r15	$E_P_1 \longrightarrow T$	
16	r16	r16	$E_P_2 \longrightarrow T$	

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
E	E	0000010
P	P	0000010

Product

Table 7: Properties of each product.

Id	Name	SBO
E_P_1	E_P_1	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

$$v_1 = \text{vol}(\text{compartment}) \cdot (k_1 \cdot [E] \cdot [P] - j_1 \cdot [E_P_1]) \quad (2)$$

6.2 Reaction r2

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

Name r2

Reaction equation



Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
E_P_1	E_P_1	0000010

Products

Table 9: Properties of each product.

Id	Name	SBO
E	E	0000011
M	M	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_2 = \text{vol}(\text{compartment}) \cdot k_2 \cdot [\text{E_P_1}] \quad (4)$$

6.3 Reaction r3

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

Name r3

Reaction equation



Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
M	M	0000010

Product

Table 11: Properties of each product.

Id	Name	SBO
M1	M1	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{compartment}) \cdot k_9 \cdot [\text{M}] \quad (6)$$

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
E	E	0000010
M1	M1	0000010

Product

Table 13: Properties of each product.

Id	Name	SBO
E_M1	E_M1	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

$$v_4 = \text{vol}(\text{compartment}) \cdot (k_3 \cdot [E] \cdot [M] - j_3 \cdot [E_M]) \quad (8)$$

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
E	E	0000010
M	M	0000010

Product

Table 15: Properties of each product.

Id	Name	SBO
E_M	E_M	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

$$v_5 = \text{vol}(\text{compartment}) \cdot (k_{3a} \cdot [E] \cdot [M] - j_{3a} \cdot [E_M]) \quad (10)$$

6.6 Reaction r6

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

Name r6

Reaction equation



Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
E_M1	E_M1	0000010

Products

Table 17: Properties of each product.

Id	Name	SBO
E	E	0000011
T	T	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_6 = \text{vol}(\text{compartment}) \cdot k_4 \cdot [\text{E_M1}] \quad (12)$$

6.7 Reaction r7

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

Name r7

Reaction equation



Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
E_M	E_M	0000010

Products

Table 19: Properties of each product.

Id	Name	SBO
E	E	0000011
T	T	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_7 = \text{vol}(\text{compartment}) \cdot k_{4a} \cdot [\text{E_M}] \quad (14)$$

6.8 Reaction r8

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

Name r8

Reaction equation



Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
E	E	0000010
P	P	0000010

Product

Table 21: Properties of each product.

Id	Name	SBO
E_P_2	E_P_2	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

$$v_8 = \text{vol}(\text{compartment}) \cdot (k_5 \cdot [E] \cdot [P] - j_5 \cdot [E_P_2]) \quad (16)$$

6.9 Reaction r9

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

Name r9

Reaction equation



Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
E_P_2	E_P_2	0000010

Products

Table 23: Properties of each product.

Id	Name	SBO
E	E	0000011
P2	P2	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_9 = \text{vol}(\text{compartment}) \cdot k_6 \cdot [E_P_2] \quad (18)$$

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
P2	P2	0000010

Product

Table 25: Properties of each product.

Id	Name	SBO
P21	P21	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_{10} = \text{vol}(\text{compartment}) \cdot k_{10} \cdot [P2] \quad (20)$$

6.11 Reaction r11

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

Name r11

Reaction equation



Reactants

Table 26: Properties of each reactant.

Id	Name	SBO
E	E	0000010
P21	P21	0000010

Product

Table 27: Properties of each product.

Id	Name	SBO
E_P21	E_P21	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

$$v_{11} = \text{vol}(\text{compartment}) \cdot (k_7 \cdot [E] \cdot [P21] - j_7 \cdot [E_P21]) \quad (22)$$

6.12 Reaction r12

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

Name r12

Reaction equation



Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
E	E	0000010
P2	P2	0000010

Product

Table 29: Properties of each product.

Id	Name	SBO
E_P2	E_P2	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

$$v_{12} = \text{vol}(\text{compartment}) \cdot (k7a \cdot [E] \cdot [P2] - j7a \cdot [E_P2]) \quad (24)$$

6.13 Reaction r13

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

Name r13

Reaction equation



Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
E_P21	E_P21	0000010

Products

Table 31: Properties of each product.

Id	Name	SBO
E	E	0000011
T	T	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_{13} = \text{vol}(\text{compartment}) \cdot k_8 \cdot [\text{E_P21}] \quad (26)$$

6.14 Reaction r14

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

Name r14

Reaction equation



Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
E_P2	E_P2	0000010

Products

Table 33: Properties of each product.

Id	Name	SBO
E	E	0000011
T	T	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_{14} = \text{vol}(\text{compartment}) \cdot k_{8a} \cdot [\text{E_P2}] \quad (28)$$

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
E_P_1	E_P_1	0000010

Product

Table 35: Properties of each product.

Id	Name	SBO
T	T	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_{15} = \text{vol}(\text{compartment}) \cdot kC1 \cdot [E_P_1] \quad (30)$$

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
E_P_2	E_P_2	0000010

Product

Table 37: Properties of each product.

Id	Name	SBO
T	T	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_{16} = \text{vol}(\text{compartment}) \cdot kC2 \cdot [E_P_2] \quad (32)$$

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 E

Name E

Initial concentration $1.5 \cdot 10^{-4} \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in twelve reactions (as a reactant in [r1](#), [r4](#), [r5](#), [r8](#), [r11](#), [r12](#) and as a product in [r2](#), [r6](#), [r7](#), [r9](#), [r13](#), [r14](#)).

$$\frac{d}{dt}E = v_2 + v_6 + v_7 + v_9 + v_{13} + v_{14} - v_1 - v_4 - v_5 - v_8 - v_{11} - v_{12} \quad (33)$$

7.2 Species E_P_1

Name E_P_1

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

This species takes part in three reactions (as a reactant in [r2](#), [r15](#) and as a product in [r1](#)).

$$\frac{d}{dt}E_P_1 = v_1 - v_2 - v_{15} \quad (34)$$

7.3 Species P

Name P

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

This species takes part in two reactions (as a reactant in [r1](#), [r8](#)).

$$\frac{d}{dt}P = -v_1 - v_8 \quad (35)$$

7.4 Species M

Name M

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

This species takes part in three reactions (as a reactant in [r3](#), [r5](#) and as a product in [r2](#)).

$$\frac{d}{dt}M = v_2 - v_3 - v_5 \quad (36)$$

7.5 Species M1

Name M1

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

This species takes part in two reactions (as a reactant in [r4](#) and as a product in [r3](#)).

$$\frac{d}{dt}M1 = v_3 - v_4 \quad (37)$$

7.6 Species E_M1

Name E_M1

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

This species takes part in two reactions (as a reactant in [r6](#) and as a product in [r4](#)).

$$\frac{d}{dt}E_M1 = v_4 - v_6 \quad (38)$$

7.7 Species E_M

Name E_M

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

This species takes part in two reactions (as a reactant in [r7](#) and as a product in [r5](#)).

$$\frac{d}{dt}E_M = v_5 - v_7 \quad (39)$$

7.8 Species T

Name T

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

This species takes part in six reactions (as a product in [r6](#), [r7](#), [r13](#), [r14](#), [r15](#), [r16](#)).

$$\frac{d}{dt}T = v_6 + v_7 + v_{13} + v_{14} + v_{15} + v_{16} \quad (40)$$

7.9 Species E_P_2

Name E_P_2

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

This species takes part in three reactions (as a reactant in [r9](#), [r16](#) and as a product in [r8](#)).

$$\frac{d}{dt}E_P_2 = v_8 - v_9 - v_{16} \quad (41)$$

7.10 Species P2

Name P2

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

This species takes part in three reactions (as a reactant in [r10](#), [r12](#) and as a product in [r9](#)).

$$\frac{d}{dt}P2 = v_9 - v_{10} - v_{12} \quad (42)$$

7.11 Species P21

Name P21

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

This species takes part in two reactions (as a reactant in [r11](#) and as a product in [r10](#)).

$$\frac{d}{dt}P21 = v_{10} - v_{11} \quad (43)$$

7.12 Species E_P21

Name E_P21

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

This species takes part in two reactions (as a reactant in [r13](#) and as a product in [r11](#)).

$$\frac{d}{dt}E_P21 = v_{11} - v_{13} \quad (44)$$

7.13 Species E_P2

Name E_P2

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

This species takes part in two reactions (as a reactant in [r14](#) and as a product in [r12](#)).

$$\frac{d}{dt}E.P2 = v_{12} - v_{14} \quad (45)$$

7.14 Species E_P1

Name E_P1

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{d}{dt}E.P1 = 0 \quad (46)$$

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: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: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.

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