**SBML Model Report**

# Model name: "Panteleev2002-_TFPImechanism_schmema1"

May 5, 2016

## 1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Michael Schubert[1] at August 26th 2011 at 4:36 p. m. and last time modified at May 28th 2014 at 4:30 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 | 8 |
| events | 0 | constraints | 0 |
| reactions | 5 | function definitions | 0 |
| global parameters | 0 | unit definitions | 2 |
| rules | 0 | initial assignments | 0 |

## 2 Unit Definitions

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

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### 2.1 Unit `time`

**Name** time

**Definition** 60 s

### 2.2 Unit `substance`

**Name** substance

**Definition** nmol

### 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 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 | ☑ | |

### 3.1 Compartment `compartment`

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

**Name** compartment

## 4 Species

This model contains eight species. Section 6 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 |
|---|---|---|---|---|---|
| VIIa_TF | VIIa_TF | compartment | $\mathrm{nmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| X | X | compartment | $\mathrm{nmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| VIIa_TF_X | VIIa_TF_X | compartment | $\mathrm{nmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| VIIa_TF_Xa | VIIa_TF_Xa | compartment | $\mathrm{nmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| Xa | Xa | compartment | $\mathrm{nmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| TFPI | TFPI | compartment | $\mathrm{nmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| Xa_TFPI | Xa_TFPI | compartment | $\mathrm{nmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| Xa_TFPI_VIIa_TF | Xa_TFPI_VIIa_TF | compartment | $\mathrm{nmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |

## 5 Reactions

This model contains five 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 4: Overview of all reactions

| № | Id | Name | Reaction Equation | SBO |
|---|---|---|---|---|
| 1 | reaction_1 | reaction_1 | $X + VIIa\_TF \rightleftharpoons VIIa\_TF\_X$ | |
| 2 | reaction_2 | reaction_2 | $VIIa\_TF\_X \longrightarrow VIIa\_TF\_Xa$ | |
| 3 | reaction_3 | reaction_3 | $VIIa\_TF\_Xa \rightleftharpoons Xa + VIIa\_TF$ | |
| 4 | reaction_4 | reaction_4 | $Xa + TFPI \rightleftharpoons Xa\_TFPI$ | |
| 5 | reaction_5 | reaction_5 | $VIIa\_TF + Xa\_TFPI \rightleftharpoons Xa\_TFPI\_VIIa\_TF$ | |

## 5.1 Reaction `reaction_1`

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

**Name** reaction_1

### Reaction equation

$$\mathrm{X} + \mathrm{VIIa\_TF} \rightleftharpoons \mathrm{VIIa\_TF\_X} \tag{1}$$

### Reactants

Table 5: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| `X` | X | 0000010 |
| `VIIa_TF` | VIIa_TF | 0000010 |

### Product

Table 6: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| `VIIa_TF_X` | VIIa_TF_X | 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

$$v_1 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k1} \cdot [\mathrm{X}] \cdot [\mathrm{VIIa\_TF}] - \mathrm{k2} \cdot [\mathrm{VIIa\_TF\_X}]) \tag{2}$$

Table 7: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| `k1` | k1 | 0000036 | 5.0 | | ☑ |
| `k2` | k2 | 0000038 | 770.0 | | ☑ |

## 5.2 Reaction reaction_2

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

**Name** reaction_2

### Reaction equation

$$\text{VIIa\_TF\_X} \longrightarrow \text{VIIa\_TF\_Xa} \tag{3}$$

### Reactant

Table 8: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| VIIa_TF_X | VIIa_TF_X | 0000010 |

### Product

Table 9: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| VIIa_TF_Xa | VIIa_TF_Xa | 0000011 |

### Kinetic Law

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

**Derived unit** contains undeclared units

$$v_2 = \text{vol}\,(\text{compartment}) \cdot \text{k1} \cdot [\text{VIIa\_TF\_X}] \tag{4}$$

Table 10: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| k1 | k1 | 0000035 | 420.0 | | ☑ |

## 5.3 Reaction reaction_3

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

**Name** reaction_3

### Reaction equation

$$\text{VIIa\_TF\_Xa} \rightleftharpoons \text{Xa} + \text{VIIa\_TF} \tag{5}$$

### Reactant

Table 11: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| VIIa_TF_Xa | VIIa_TF_Xa | 0000010 |

### Products

Table 12: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| Xa | Xa | 0000011 |
| VIIa_TF | VIIa_TF | 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

$$v_3 = \text{vol}\,(\text{compartment}) \cdot (\text{k1} \cdot [\text{VIIa\_TF\_Xa}] - \text{k2} \cdot [\text{Xa}] \cdot [\text{VIIa\_TF}]) \tag{6}$$

Table 13: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| k1 | k1 | 0000035 | 770.0 | | ☑ |
| k2 | k2 | 0000039 | 5.0 | | ☑ |

## 5.4 Reaction reaction_4

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

**Name** reaction_4

### Reaction equation

$$\mathrm{Xa} + \mathrm{TFPI} \rightleftharpoons \mathrm{Xa\_TFPI} \tag{7}$$

### Reactants

Table 14: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| Xa | Xa | 0000010 |
| TFPI | TFPI | 0000010 |

### Product

Table 15: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| Xa_TFPI | Xa_TFPI | 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

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k1} \cdot [\mathrm{Xa}] \cdot [\mathrm{TFPI}] - \mathrm{k2} \cdot [\mathrm{Xa\_TFPI}]) \tag{8}$$

Table 16: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| k1 | k1 | 0000036 | 0.054 | | ☑ |
| k2 | k2 | 0000038 | 0.020 | | ☑ |

## 5.5 Reaction reaction_5

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

**Name** reaction_5

### Reaction equation

$$\text{VIIa\_TF} + \text{Xa\_TFPI} \rightleftharpoons \text{Xa\_TFPI\_VIIa\_TF} \tag{9}$$

### Reactants

Table 17: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| VIIa_TF | VIIa_TF | 0000010 |
| Xa_TFPI | Xa_TFPI | 0000010 |

### Product

Table 18: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| Xa_TFPI_VIIa_TF | Xa_TFPI_VIIa_TF | 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

$$v_5 = \text{vol}\,(\text{compartment}) \cdot (\text{k1} \cdot [\text{VIIa\_TF}] \cdot [\text{Xa\_TFPI}] - \text{k2} \cdot [\text{Xa\_TFPI\_VIIa\_TF}]) \tag{10}$$

Table 19: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| k1 | k1 | 0000036 | 0.440 | | ☑ |
| k2 | k2 | 0000038 | 0.066 | | ☑ |

## 6 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.

## 6.1 Species `VIIa_TF`

**Name** VIIa_TF

**Initial concentration** $0.9999997\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in `reaction_1`, `reaction_5` and as a product in `reaction_3`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{VIIa\_TF} = v_3 - v_1 - v_5 \tag{11}$$

## 6.2 Species `X`

**Name** X

**Initial concentration** $169.9999\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in `reaction_1`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = -v_1 \tag{12}$$

## 6.3 Species `VIIa_TF_X`

**Name** VIIa_TF_X

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

This species takes part in two reactions (as a reactant in `reaction_2` and as a product in `reaction_1`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{VIIa\_TF\_X} = v_1 - v_2 \tag{13}$$

## 6.4 Species `VIIa_TF_Xa`

**Name** VIIa_TF_Xa

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

This species takes part in two reactions (as a reactant in `reaction_3` and as a product in `reaction_2`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{VIIa\_TF\_Xa} = v_2 - v_3 \tag{14}$$

## 6.5 Species Xa

**Name** Xa

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

This species takes part in two reactions (as a reactant in reaction_4 and as a product in reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xa} = v_3 - v_4 \tag{15}$$

## 6.6 Species TFPI

**Name** TFPI

**Initial concentration** $2.399999\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in reaction_4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TFPI} = -v_4 \tag{16}$$

## 6.7 Species Xa_TFPI

**Name** Xa_TFPI

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

This species takes part in two reactions (as a reactant in reaction_5 and as a product in reaction_4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xa\_TFPI} = v_4 - v_5 \tag{17}$$

## 6.8 Species Xa_TFPI_VIIa_TF

**Name** Xa_TFPI_VIIa_TF

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

This species takes part in one reaction (as a product in reaction_5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xa\_TFPI\_VIIa\_TF} = v_5 \tag{18}$$

## 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.

SBML2LaTeX 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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