

SBML Model Report

Model name: “Yang2007_ArachidonicAcid”



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Enuo He¹ and Kun Yang² at January twelveth 2007 at 3:06 p.m. and last time modified at July fifth 2012 at 2:48 p.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 | 1 |
| species types | 0 | species | 25 |
| events | 0 | constraints | 0 |
| reactions | 32 | function definitions | 0 |
| global parameters | 54 | unit definitions | 2 |
| rules | 0 | initial assignments | 0 |

Model Notes

This model is according to the paper *Dynamic Simulation on the Arachidonic Acid Metabolic Network*. Figure 2A has been reproduced by SBML ode solver on line. In the original model, all the reactions are presented as ODE directly. So curator rewrite each reaction according to the semantics of the paper. In this paper, the authors used quick complex kinetics law to describe the catalysis in the network, curators did not necessarily know all the complete meanings of the

¹BNMC, enuo@caltech.edu

²Beijing National Laboratory for Molecular Sciences

paper.

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To cite BioModels Database, please use: [Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C \(2010\) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.](#)

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 micromole

Definition μmol

2.2 Unit time

Name minute

Definition 60 s

2.3 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

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 |
|------|------|-----|-----------------------|------|-------|-------------------------------------|---------|
| cell | cell | | 3 | 1 | litre | <input checked="" type="checkbox"/> | |

3.1 Compartment `cell`

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

Name `cell`

4 Species

This model contains 25 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 |
|-----|----------|-------------|-------------------------------------|-----------|--------------------|
| x1 | AA | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x10 | 5-HPETE | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x11 | 5-HETE | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x12 | LTA4 | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x13 | LTB4 | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x14 | w-LTB4 | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x15 | PLA2 | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x16 | 15-LOX | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x17 | 12-LOX | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x18 | COX-2 | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x19 | PGES | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x2 | 15-HPETE | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x20 | TXAS | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x21 | 5-LOX | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x22 | LTA4H | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x23 | CYP4F3 | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x24 | PHGPx | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x25 | exo-AA | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x3 | 15-HETE | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x4 | 12-HPETE | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x5 | 12-HETE | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| x6 | PGH2 | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | \square | \square |

| Id | Name | Compartment | Derived Unit | Constant | Boundary Condi- tion |
|----|------|-------------|-------------------------------------|--------------------------|----------------------------|
| x7 | PGE2 | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/> |
| x8 | TXA2 | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/> |
| x9 | TXB2 | cell | $\mu\text{mol} \cdot \text{l}^{-1}$ | <input type="checkbox"/> | <input type="checkbox"/> |

5 Parameters

This model contains 54 global parameters.

Table 4: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|------|--------------|-----|----------|------|-------------------------------------|
| lin | lin | | 12.000 | | <input checked="" type="checkbox"/> |
| K15 | Kcat(PLA2) | | 3600.000 | | <input checked="" type="checkbox"/> |
| k15 | Km(PLA2) | | 2600.000 | | <input checked="" type="checkbox"/> |
| K16 | Kcat(15-LOX) | | 1000.000 | | <input checked="" type="checkbox"/> |
| k16 | Km(15-LOX) | | 70.000 | | <input checked="" type="checkbox"/> |
| K17 | Kcat(12-LOX) | | 1000.000 | | <input checked="" type="checkbox"/> |
| k17 | Km(12-LOX) | | 50.000 | | <input checked="" type="checkbox"/> |
| K18 | Kcat(COX-2) | | 1000.000 | | <input checked="" type="checkbox"/> |
| k18 | Km(COX-2) | | 50.000 | | <input checked="" type="checkbox"/> |
| K19 | Kcat(PGES) | | 3000.000 | | <input checked="" type="checkbox"/> |
| k19 | Km(PGES) | | 160.000 | | <input checked="" type="checkbox"/> |
| K20 | Kcat(TXAS) | | 1599.000 | | <input checked="" type="checkbox"/> |
| k20 | Km(TXAS) | | 4.000 | | <input checked="" type="checkbox"/> |
| K21 | Kcat(5-LOX) | | 5000.000 | | <input checked="" type="checkbox"/> |
| k21 | Km(5-LOX) | | 5.000 | | <input checked="" type="checkbox"/> |
| K22 | Kcat(LTA4H) | | 125.000 | | <input checked="" type="checkbox"/> |
| k22 | Km(LTA4H) | | 20.000 | | <input checked="" type="checkbox"/> |
| K23 | Kcat(CYP4F3) | | 150.000 | | <input checked="" type="checkbox"/> |
| k23 | Km(CYP4F3) | | 3.900 | | <input checked="" type="checkbox"/> |
| K24 | Kcat(PHGPx) | | 500.000 | | <input checked="" type="checkbox"/> |
| k24 | Km(PHGPx) | | 70.000 | | <input checked="" type="checkbox"/> |
| kd2 | | | 0.050 | | <input checked="" type="checkbox"/> |
| kd3 | | | 0.010 | | <input checked="" type="checkbox"/> |
| kd8 | | | 0.100 | | <input checked="" type="checkbox"/> |
| kd9 | | | 0.001 | | <input checked="" type="checkbox"/> |
| kd11 | | | 0.001 | | <input checked="" type="checkbox"/> |
| kd12 | | | 0.070 | | <input checked="" type="checkbox"/> |
| kd13 | | | 0.010 | | <input checked="" type="checkbox"/> |
| kd16 | | | 0.010 | | <input checked="" type="checkbox"/> |
| ki1 | | | 0.300 | | <input checked="" type="checkbox"/> |
| ki2 | | | 30.000 | | <input checked="" type="checkbox"/> |
| ki3 | | | 30.000 | | <input checked="" type="checkbox"/> |
| ki4 | | | 0.600 | | <input checked="" type="checkbox"/> |
| ki5 | | | 0.100 | | <input checked="" type="checkbox"/> |
| ki6 | | | 0.010 | | <input checked="" type="checkbox"/> |
| ki7 | | | 30.000 | | <input checked="" type="checkbox"/> |
| ki8 | | | 4.000 | | <input checked="" type="checkbox"/> |

| Id | Name | SBO | Value | Unit | Constant |
|------|------|-----|---------------------|------|-------------------------------------|
| ki9 | | | 0.175 | | <input checked="" type="checkbox"/> |
| ki10 | | | 0.010 | | <input checked="" type="checkbox"/> |
| ki11 | | | 15.000 | | <input checked="" type="checkbox"/> |
| ki12 | | | 6.300 | | <input checked="" type="checkbox"/> |
| ki14 | | | 0.200 | | <input checked="" type="checkbox"/> |
| ki15 | | | 0.860 | | <input checked="" type="checkbox"/> |
| ki16 | | | 10.000 | | <input checked="" type="checkbox"/> |
| ki17 | | | 10.000 | | <input checked="" type="checkbox"/> |
| ki18 | | | 10.000 | | <input checked="" type="checkbox"/> |
| KI19 | | | 500.000 | | <input checked="" type="checkbox"/> |
| KI20 | | | 200.000 | | <input checked="" type="checkbox"/> |
| KI21 | | | 500.000 | | <input checked="" type="checkbox"/> |
| KI22 | | | 500.000 | | <input checked="" type="checkbox"/> |
| KI23 | | | 0.053 | | <input checked="" type="checkbox"/> |
| KI24 | | | $2.3 \cdot 10^{-5}$ | | <input checked="" type="checkbox"/> |
| a24 | | | 0.150 | | <input checked="" type="checkbox"/> |
| ks | | | 500.000 | | <input checked="" type="checkbox"/> |

6 Reactions

This model contains 32 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 | AA production | $\emptyset \xrightarrow{x11, x13, x15, x2, x4} x1$ | |
| 2 | R2 | 15-HPETE production | $x1 \xrightleftharpoons{x16} x2$ | |
| 3 | R3 | 15-HETE production | $x2 \xrightleftharpoons{x24} x3$ | |
| 4 | R4 | 12-HPETE production | $x1 \xrightleftharpoons{x17, x3} x4$ | |
| 5 | R5 | 12-HETE production | $x4 \xrightleftharpoons{x24} x5$ | |
| 6 | R6 | PGH2 production | $x1 \xrightleftharpoons{x18, x7} x6$ | |
| 7 | R7 | PGE2 production | $x6 \xrightleftharpoons{x1, x19, x3} x7$ | |
| 8 | R8 | TXA2 production | $x6 \xrightleftharpoons{x20} x8$ | |
| 9 | R9 | TXB2 production | $\emptyset \xrightarrow{x8} x9$ | |
| 10 | R10 | 5-HPETE production | $x1 \xrightleftharpoons{x11, x3, x5, x7, x21} x10$ | |
| 11 | R11 | 5-HETE production | $x10 \xrightleftharpoons{x24} x11$ | |
| 12 | R12 | LTA4 production | $x10 \xrightleftharpoons{x11, x21, x3, x5, x7} x12$ | |
| 13 | R13 | LTB4 production | $x12 \xrightleftharpoons{x22} x13$ | |
| 14 | R14 | 20-OH-LTB4 production | $x13 \xrightleftharpoons{x11, x23, x5} x14$ | |
| 15 | R16 | 15-LOX upregulation | $\emptyset \xrightarrow{x7} x16$ | |
| 16 | R17 | 12-LOX inhibition | $x17 \xrightarrow{x2} \emptyset$ | |

| Nº | Id | Name | Reaction Equation | SBO |
|----|-----|-------------------------|---|-----|
| 17 | R20 | TXAS inhibition | $x_{20} \xrightarrow{x_2} \emptyset$ | |
| 18 | R21 | 5-LOX upregulation | $\emptyset \xrightarrow{x_{13}} x_{21}$ | |
| 19 | R22 | LTA4H inhibition | $x_{22} \xrightarrow{x_{12}} \emptyset$ | |
| 20 | R18 | TXB2 decay | $x_9 \longrightarrow \emptyset$ | |
| 21 | R19 | TXAS inhibition by PGH2 | $x_{20} \xrightarrow{x_6} \emptyset$ | |
| 22 | R25 | TAX2 decay | $x_8 \longrightarrow \emptyset$ | |
| 23 | R24 | LTB4 decay | $x_{13} \longrightarrow \emptyset$ | |
| 24 | R23 | LTA4 decay | $x_{12} \longrightarrow \emptyset$ | |
| 25 | R26 | 15-HETE decay | $x_3 \longrightarrow \emptyset$ | |
| 26 | R27 | 15-HPETE decay | $x_2 \longrightarrow \emptyset$ | |
| 27 | R28 | 15-LOX decay | $x_{16} \longrightarrow \emptyset$ | |
| 28 | R29 | 5-HETE decay | $x_{11} \longrightarrow \emptyset$ | |
| 29 | R30 | 5-LOX inhibition by x12 | $x_{21} \xrightarrow{x_{12}} \emptyset$ | |
| 30 | R31 | 5-LOX inhibition by x10 | $x_{21} \xrightarrow{x_{10}} \emptyset$ | |
| 31 | R32 | 5-LOX inhibition by x2 | $x_{21} \xrightarrow{x_2} \emptyset$ | |
| 32 | R34 | AA decay | $x_1 \longrightarrow \emptyset$ | |

6.1 Reaction R1

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

Name AA production

Reaction equation



Modifiers

Table 6: Properties of each modifier.

| Id | Name | SBO |
|-----|----------|-----|
| x11 | 5-HETE | |
| x13 | LTB4 | |
| x15 | PLA2 | |
| x2 | 15-HPETE | |
| x4 | 12-HPETE | |

Product

Table 7: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| x1 | AA | |

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\text{vol}(\text{cell}) \cdot K15 \cdot [x15] \cdot \text{lin} \cdot \left(1 + \frac{[x4]}{KI19} + \frac{[x2]}{KI20} + \frac{[x13]}{KI21} + \frac{[x11]}{KI22}\right)}{\text{lin} + k15 \cdot \left(1 + \frac{[x1]}{ks}\right)} \quad (2)$$

6.2 Reaction R2

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name 15-HPETE production

Reaction equation



Reactant

Table 8: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| x1 | AA | |

Modifier

Table 9: Properties of each modifier.

| Id | Name | SBO |
|-----|--------|-----|
| x16 | 15-LOX | |

Product

Table 10: Properties of each product.

| Id | Name | SBO |
|----|----------|-----|
| x2 | 15-HPETE | |

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\text{vol}(\text{cell}) \cdot K16 \cdot [x16] \cdot [x1]}{[x1] + k16 \cdot \left(1 + \frac{[x2]}{k_s}\right)} \quad (4)$$

6.3 Reaction R3

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name 15-HETE production

Reaction equation



Reactant

Table 11: Properties of each reactant.

| Id | Name | SBO |
|----|----------|-----|
| x2 | 15-HPETE | |

Modifier

Table 12: Properties of each modifier.

| Id | Name | SBO |
|-----|-------|-----|
| x24 | PHGPx | |

Product

Table 13: Properties of each product.

| Id | Name | SBO |
|----|---------|-----|
| x3 | 15-HETE | |

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\text{vol}(\text{cell}) \cdot K_{24} \cdot [x_{24}] \cdot [x_2]}{[x_2] + k_{24} \cdot \left(1 + \frac{[x_3]}{k_s}\right)} \quad (6)$$

6.4 Reaction R4

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name 12-HPETE production

Reaction equation



Reactant

Table 14: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| x1 | AA | |

Modifiers

Table 15: Properties of each modifier.

| Id | Name | SBO |
|-----|---------|-----|
| x17 | 12-LOX | |
| x3 | 15-HETE | |

Product

Table 16: Properties of each product.

| Id | Name | SBO |
|----|----------|-----|
| x4 | 12-HPETE | |

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \frac{\text{vol}(\text{cell}) \cdot K17 \cdot [x17] \cdot [x1]}{[x1] + k17 \cdot \left(1 + \frac{[x4]}{ki18} + \frac{[x3]}{ki16} + \frac{[x4]}{ks}\right)} \quad (8)$$

6.5 Reaction R5

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name 12-HETE production

Reaction equation



Reactant

Table 17: Properties of each reactant.

| Id | Name | SBO |
|----|----------|-----|
| x4 | 12-HPETE | |

Modifier

Table 18: Properties of each modifier.

| Id | Name | SBO |
|-----|-------|-----|
| x24 | PHGPx | |

Product

Table 19: Properties of each product.

| Id | Name | SBO |
|----|---------|-----|
| x5 | 12-HETE | |

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\text{vol}(\text{cell}) \cdot K_{24} \cdot [x_{24}] \cdot [x_4]}{[x_4] + k_{24} \cdot \left(1 + \frac{[x_5]}{k_s}\right)} \quad (10)$$

6.6 Reaction R6

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name PGH2 production

Reaction equation



Reactant

Table 20: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| x1 | AA | |

Modifiers

Table 21: Properties of each modifier.

| Id | Name | SBO |
|-----|-------|-----|
| x18 | COX-2 | |
| x7 | PGE2 | |

Product

Table 22: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| x6 | PGH2 | |

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \frac{\text{vol}(\text{cell}) \cdot K18 \cdot [x18] \cdot [x1]}{[x1] + k18 \cdot \left(1 + \frac{[x7]}{ki3} + \frac{[x6]}{ks}\right)} \quad (12)$$

6.7 Reaction R7

This is a reversible reaction of one reactant forming one product influenced by three modifiers.

Name PGE2 production

Reaction equation



Reactant

Table 23: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| x6 | PGH2 | |

Modifiers

Table 24: Properties of each modifier.

| Id | Name | SBO |
|-----|---------|-----|
| x1 | AA | |
| x19 | PGES | |
| x3 | 15-HETE | |

Product

Table 25: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| x7 | PGE2 | |

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\text{vol}(\text{cell}) \cdot K19 \cdot [x19] \cdot [x6]}{[x6] + k19 \cdot \left(1 + \frac{[x1]}{ki1} + \frac{[x3]}{ki2} + \frac{[x7]}{ks}\right)} \quad (14)$$

6.8 Reaction R8

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name TXA2 production

Reaction equation



Reactant

Table 26: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| x6 | PGH2 | |

Modifier

Table 27: Properties of each modifier.

| Id | Name | SBO |
|-----|------|-----|
| x20 | TXAS | |

Product

Table 28: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| x8 | TXA2 | |

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\text{vol}(\text{cell}) \cdot K_{20} \cdot [x_{20}] \cdot [x_6]}{[x_6] + k_{20} \cdot \left(1 + \frac{[x_8]}{k_s}\right)} \quad (16)$$

6.9 Reaction R9

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

Name TXB2 production

Reaction equation



Modifier

Table 29: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| x8 | TXA2 | |

Product

Table 30: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| x9 | TXB2 | |

Kinetic Law

Derived unit contains undeclared units

$$v_9 = kd8 \cdot [x8] \cdot \text{vol}(\text{cell}) \quad (18)$$

6.10 Reaction R10

This is a reversible reaction of one reactant forming one product influenced by five modifiers.

Name 5-HPETE production

Reaction equation



Reactant

Table 31: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| x1 | AA | |

Modifiers

Table 32: Properties of each modifier.

| Id | Name | SBO |
|-----|--------|-----|
| x11 | 5-HETE | |

| Id | Name | SBO |
|-----|---------|-----|
| x3 | 15-HETE | |
| x5 | 12-HETE | |
| x7 | PGE2 | |
| x21 | 5-LOX | |

Product

Table 33: Properties of each product.

| Id | Name | SBO |
|-----|---------|-----|
| x10 | 5-HPETE | |

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \frac{\text{vol}(\text{cell}) \cdot K_{21} \cdot [x_{21}] \cdot [x_1]}{[x_1] + k_{21} \cdot \left(1 + \frac{[x_5]}{k_{i7}} + \frac{[x_3]}{k_{i8}} + \frac{[x_7]}{k_{i11}} + \frac{[x_{11}]}{k_{i12}} + \frac{[x_{10}]}{k_s}\right)} \quad (20)$$

6.11 Reaction R11

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name 5-HETE production

Reaction equation



Reactant

Table 34: Properties of each reactant.

| Id | Name | SBO |
|-----|---------|-----|
| x10 | 5-HPETE | |

Modifier

Table 35: Properties of each modifier.

| Id | Name | SBO |
|-----|-------|-----|
| x24 | PHGPx | |

Product

Table 36: Properties of each product.

| Id | Name | SBO |
|-----|--------|-----|
| x11 | 5-HETE | |

Kinetic Law

Derived unit contains undeclared units

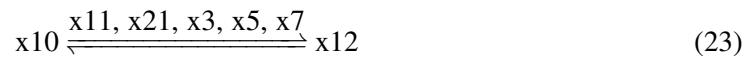
$$v_{11} = \frac{\text{vol}(\text{cell}) \cdot K24 \cdot [x24] \cdot [x10]}{[x10] + k24 \cdot \left(1 + \frac{[x11]}{k_s}\right)} \quad (22)$$

6.12 Reaction R12

This is a reversible reaction of one reactant forming one product influenced by five modifiers.

Name LTA4 production

Reaction equation



Reactant

Table 37: Properties of each reactant.

| Id | Name | SBO |
|-----|---------|-----|
| x10 | 5-HPETE | |

Modifiers

Table 38: Properties of each modifier.

| Id | Name | SBO |
|-----|---------|-----|
| x11 | 5-HETE | |
| x21 | 5-LOX | |
| x3 | 15-HETE | |
| x5 | 12-HETE | |
| x7 | PGE2 | |

Product

Table 39: Properties of each product.

| Id | Name | SBO |
|-----|------|-----|
| x12 | LTA4 | |

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \frac{\text{vol}(\text{cell}) \cdot K_{21} \cdot [x_{21}] \cdot [x_{10}]}{[x_{10}] + k_{21} \cdot \left(1 + \frac{[x_5]}{k_{i7}} + \frac{[x_3]}{k_{i8}} + \frac{[x_7]}{k_{i11}} + \frac{[x_{11}]}{k_{i12}} + \frac{[x_{12}]}{k_s} \right)} \quad (24)$$

6.13 Reaction R13

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name LTB4 production

Reaction equation



Reactant

Table 40: Properties of each reactant.

| Id | Name | SBO |
|-----|------|-----|
| x12 | LTA4 | |

Modifier

Table 41: Properties of each modifier.

| Id | Name | SBO |
|-----|-------|-----|
| x22 | LTA4H | |

Product

Table 42: Properties of each product.

| Id | Name | SBO |
|-----|------|-----|
| x13 | LTB4 | |

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \frac{\text{vol}(\text{cell}) \cdot K_{22} \cdot [x_{22}] \cdot [x_{12}]}{[x_{12}] + k_{22} \cdot \left(1 + \frac{[x_{13}]}{k_s}\right)} \quad (26)$$

6.14 Reaction R14

This is a reversible reaction of one reactant forming one product influenced by three modifiers.

Name 20-OH-LTB4 production

Reaction equation



Reactant

Table 43: Properties of each reactant.

| Id | Name | SBO |
|-----|------|-----|
| x13 | LTB4 | |

Modifiers

Table 44: Properties of each modifier.

| Id | Name | SBO |
|-----|---------|-----|
| x11 | 5-HETE | |
| x23 | CYP4F3 | |
| x5 | 12-HETE | |

Product

Table 45: Properties of each product.

| Id | Name | SBO |
|-----|--------|-----|
| x14 | w-LTB4 | |

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \frac{\text{vol}(\text{cell}) \cdot K_{23} \cdot [x_{23}] \cdot [x_{13}]}{[x_{13}] + k_{23} \cdot \left(1 + \frac{[x_5]}{k_{i14}} + \frac{[x_{11}]}{k_{i15}} + \frac{[x_{14}]}{k_s}\right)} \quad (28)$$

6.15 Reaction R16

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

Name 15-LOX upregulation

Reaction equation



Modifier

Table 46: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| x7 | PGE2 | |

Product

Table 47: Properties of each product.

| Id | Name | SBO |
|-----|--------|-----|
| x16 | 15-LOX | |

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \frac{\text{vol}(\text{cell}) \cdot a_{24} \cdot [x7] \cdot [x7]}{[x7] \cdot [x7] + KI_{24} \cdot KI_{24}} \quad (30)$$

6.16 Reaction R17

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

Name 12-LOX inhibition

Reaction equation



Reactant

Table 48: Properties of each reactant.

| Id | Name | SBO |
|-----|--------|-----|
| x17 | 12-LOX | |

Modifier

Table 49: Properties of each modifier.

| Id | Name | SBO |
|----|----------|-----|
| x2 | 15-HPETE | |

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{vol}(\text{cell}) \cdot ki_{17} \cdot [x2] \cdot [x17] \quad (32)$$

6.17 Reaction R20

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

Name TXAS inhibition

Reaction equation



Reactant

Table 50: Properties of each reactant.

| Id | Name | SBO |
|-----|------|-----|
| x20 | TXAS | |

Modifier

Table 51: Properties of each modifier.

| Id | Name | SBO |
|----|----------|-----|
| x2 | 15-HPETE | |

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = ki4 \cdot [x2] \cdot [x20] \cdot vol (cell)$$

(34)

6.18 Reaction R21

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

Name 5-LOX upregulation

Reaction equation



Modifier

Table 52: Properties of each modifier.

| Id | Name | SBO |
|-----|------|-----|
| x13 | LTB4 | |

Product

Table 53: Properties of each product.

| Id | Name | SBO |
|-----|-------|-----|
| x21 | 5-LOX | |

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol}(\text{cell}) \cdot \text{KI23} \cdot [\text{x13}] \cdot [\text{x21}] \quad (36)$$

6.19 Reaction R22

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

Name LTA4H inhibition

Reaction equation



Reactant

Table 54: Properties of each reactant.

| Id | Name | SBO |
|-----|-------|-----|
| x22 | LTA4H | |

Modifier

Table 55: Properties of each modifier.

| Id | Name | SBO |
|-----|------|-----|
| x12 | LTA4 | |

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \frac{\text{vol}(\text{cell}) \cdot K_{22} \cdot [x_{22}] \cdot [x_{12}]}{([x_{12}] + k_{22}) \cdot 129} \quad (38)$$

6.20 Reaction R18

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

Name TXB2 decay

Reaction equation



Reactant

Table 56: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| x9 | TXB2 | |

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = k_{d9} \cdot [x_9] \cdot \text{vol}(\text{cell}) \quad (40)$$

6.21 Reaction R19

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

Name TXAS inhibition by PGH2

Reaction equation



Reactant

Table 57: Properties of each reactant.

| Id | Name | SBO |
|-----|------|-----|
| x20 | TXAS | |

Modifier

Table 58: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| x6 | PGH2 | |

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{vol}(\text{cell}) \cdot \text{ki5} \cdot [\text{x6}] \cdot [\text{x20}] \quad (42)$$

6.22 Reaction R25

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

Name TAX2 decay

Reaction equation



Reactant

Table 59: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| x8 | TXA2 | |

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{vol}(\text{cell}) \cdot \text{kd8} \cdot [\text{x8}] \quad (44)$$

6.23 Reaction R24

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

Name LTB4 decay

Reaction equation



Reactant

Table 60: Properties of each reactant.

| Id | Name | SBO |
|-----|------|-----|
| x13 | LTB4 | |

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{vol}(\text{cell}) \cdot \text{kd13} \cdot [x13]$$

(46)

6.24 Reaction R23

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

Name LTA4 decay

Reaction equation



Reactant

Table 61: Properties of each reactant.

| Id | Name | SBO |
|-----|------|-----|
| x12 | LTA4 | |

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \text{vol}(\text{cell}) \cdot [x12] \cdot \text{kd12}$$

(48)

6.25 Reaction R26

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

Name 15-HETE decay

Reaction equation



Reactant

Table 62: Properties of each reactant.

| Id | Name | SBO |
|----|---------|-----|
| x3 | 15-HETE | |

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = kd3 \cdot [x3] \cdot vol(\text{cell}) \quad (50)$$

6.26 Reaction R27

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

Name 15-HPETE decay

Reaction equation



Reactant

Table 63: Properties of each reactant.

| Id | Name | SBO |
|----|----------|-----|
| x2 | 15-HPETE | |

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = kd2 \cdot vol(\text{cell}) \cdot [x2] \quad (52)$$

6.27 Reaction R28

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

Name 15-LOX decay

Reaction equation



Reactant

Table 64: Properties of each reactant.

| Id | Name | SBO |
|-----|--------|-----|
| x16 | 15-LOX | |

Kinetic Law

Derived unit contains undeclared units

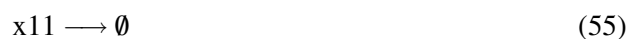
$$v_{27} = \text{vol}(\text{cell}) \cdot \text{kd16} \cdot [x16] \quad (54)$$

6.28 Reaction R29

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

Name 5-HETE decay

Reaction equation



Reactant

Table 65: Properties of each reactant.

| Id | Name | SBO |
|-----|--------|-----|
| x11 | 5-HETE | |

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \text{kd11} \cdot [x11] \cdot \text{vol}(\text{cell}) \quad (56)$$

6.29 Reaction R30

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

Name 5-LOX inhibition by x12

Reaction equation



Reactant

Table 66: Properties of each reactant.

| Id | Name | SBO |
|-----|-------|-----|
| x21 | 5-LOX | |

Modifier

Table 67: Properties of each modifier.

| Id | Name | SBO |
|-----|------|-----|
| x12 | LTA4 | |

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \text{vol}(\text{cell}) \cdot k_{i9} \cdot [x_{12}] \cdot [x_{21}] \quad (58)$$

6.30 Reaction R31

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

Name 5-LOX inhibition by x10

Reaction equation



Reactant

Table 68: Properties of each reactant.

| Id | Name | SBO |
|-----|-------|-----|
| x21 | 5-LOX | |

Modifier

Table 69: Properties of each modifier.

| Id | Name | SBO |
|-----|---------|-----|
| x10 | 5-HPETE | |

Kinetic Law**Derived unit** contains undeclared units

$$v_{30} = \text{vol}(\text{cell}) \cdot \text{ki10} \cdot [\text{x10}] \cdot [\text{x21}] \quad (60)$$

6.31 Reaction R32

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

Name 5-LOX inhibition by x2**Reaction equation****Reactant**

Table 70: Properties of each reactant.

| Id | Name | SBO |
|-----|-------|-----|
| x21 | 5-LOX | |

Modifier

Table 71: Properties of each modifier.

| Id | Name | SBO |
|----|----------|-----|
| x2 | 15-HPETE | |

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \text{vol}(\text{cell}) \cdot \text{ki6} \cdot [\text{x21}] \cdot [\text{x2}] \quad (62)$$

6.32 Reaction R34

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

Name AA decay

Reaction equation



Reactant

Table 72: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| x1 | AA | |

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = 0.1 \cdot [\text{x1}] \cdot \text{vol}(\text{cell}) \quad (64)$$

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 x1

Name AA

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in R2, R4, R6, R10, R34 and as a product in R1 and as a modifier in R7).

$$\frac{d}{dt}x1 = v_1 - v_2 - v_4 - v_6 - v_{10} - v_{32} \quad (65)$$

7.2 Species x10

Name 5-HPETE

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in R11, R12 and as a product in R10 and as a modifier in R31).

$$\frac{d}{dt}x10 = v_{10} - v_{11} - v_{12} \quad (66)$$

7.3 Species x11

Name 5-HETE

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in R29 and as a product in R11 and as a modifier in R1, R10, R12, R14).

$$\frac{d}{dt}x11 = v_{11} - v_{28} \quad (67)$$

7.4 Species x12

Name LTA4

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in R13, R23 and as a product in R12 and as a modifier in R22, R30).

$$\frac{d}{dt}x12 = v_{12} - v_{13} - v_{24} \quad (68)$$

7.5 Species x13

Name LTB4

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [R14](#), [R24](#) and as a product in [R13](#) and as a modifier in [R1](#), [R21](#)).

$$\frac{d}{dt}x_{13} = v_{13} - v_{14} - v_{23} \quad (69)$$

7.6 Species x14

Name w-LTB4

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R14](#)).

$$\frac{d}{dt}x_{14} = v_{14} \quad (70)$$

7.7 Species x15

Name PLA2

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

This species takes part in one reaction (as a modifier in [R1](#)).

$$\frac{d}{dt}x_{15} = 0 \quad (71)$$

7.8 Species x16

Name 15-LOX

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

This species takes part in three reactions (as a reactant in [R28](#) and as a product in [R16](#) and as a modifier in [R2](#)).

$$\frac{d}{dt}x_{16} = v_{15} - v_{27} \quad (72)$$

7.9 Species x17

Name 12-LOX

Initial concentration $0.5 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in R17 and as a modifier in R4).

$$\frac{d}{dt}x17 = -v16 \quad (73)$$

7.10 Species x18

Name COX-2

Initial concentration $0.2 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in R6).

$$\frac{d}{dt}x18 = 0 \quad (74)$$

7.11 Species x19

Name PGES

Initial concentration $0.5 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in R7).

$$\frac{d}{dt}x19 = 0 \quad (75)$$

7.12 Species x2

Name 15-HPETE

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in R3, R27 and as a product in R2 and as a modifier in R1, R17, R20, R32).

$$\frac{d}{dt}x2 = v2 - v3 - v26 \quad (76)$$

7.13 Species x20

Name TXAS

Initial concentration $0.5 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R20, R19 and as a modifier in R8).

$$\frac{d}{dt}x20 = -v17 - v21 \quad (77)$$

7.14 Species x21

Name 5-LOX

Initial concentration $5 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in [R30](#), [R31](#), [R32](#) and as a product in [R21](#) and as a modifier in [R10](#), [R12](#)).

$$\frac{d}{dt}x_{21} = v_{18} - v_{29} - v_{30} - v_{31} \quad (78)$$

7.15 Species x22

Name LTA4H

Initial concentration $0.76 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [R22](#) and as a modifier in [R13](#)).

$$\frac{d}{dt}x_{22} = -v_{19} \quad (79)$$

7.16 Species x23

Name CYP4F3

Initial concentration $0.07 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in [R14](#)).

$$\frac{d}{dt}x_{23} = 0 \quad (80)$$

7.17 Species x24

Name PHGPx

Initial concentration $0.8 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a modifier in [R3](#), [R5](#), [R11](#)).

$$\frac{d}{dt}x_{24} = 0 \quad (81)$$

7.18 Species x25

Name exo-AA

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:

$$\frac{d}{dt}x_{25} = 0 \quad (82)$$

7.19 Species x3

Name 15-HETE

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in R26 and as a product in R3 and as a modifier in R4, R7, R10, R12).

$$\frac{d}{dt}x_3 = v_3 - v_{25} \quad (83)$$

7.20 Species x4

Name 12-HPETE

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R5 and as a product in R4 and as a modifier in R1).

$$\frac{d}{dt}x_4 = v_4 - v_5 \quad (84)$$

7.21 Species x5

Name 12-HETE

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a product in R5 and as a modifier in R10, R12, R14).

$$\frac{d}{dt}x_5 = v_5 \quad (85)$$

7.22 Species x6

Name PGH2

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in R7, R8 and as a product in R6 and as a modifier in R19).

$$\frac{d}{dt}x_6 = v_6 - v_7 - v_8 \quad (86)$$

7.23 Species x7

Name PGE2

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a product in R7 and as a modifier in R6, R10, R12, R16).

$$\frac{d}{dt}x7 = v7 \quad (87)$$

7.24 Species x8

Name TXA2

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R25 and as a product in R8 and as a modifier in R9).

$$\frac{d}{dt}x8 = v8 - v22 \quad (88)$$

7.25 Species x9

Name TXB2

Initial concentration $0.0010 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in R18 and as a product in R9).

$$\frac{d}{dt}x9 = v9 - v20 \quad (89)$$

SBML2^{LaTeX} 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