SBML Model Report

Model name: "Gupta2009 - Eicosanoid Metabolism"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following six authors: Byrnes Robert[1], Shakti Gupta[2], Mano Ram Maurya[3], Daren L. Stephens[4], Edward A. Dennis[5] and Shankar Subramaniam[6] at January 22nd 2010 at 10:59 p. m. and last time modified at December eleventh 2012 at 7:15 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	13
events	7	constraints	0
reactions	22	function definitions	1
global parameters	77	unit definitions	7
rules	4	initial assignments	0

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Model Notes

Gupta2009 - Eicosanoid Metabolism

Integrated model of eicosanoid metabolism and signaling based on lipidomics flux analysis.

This model is described in the article:An integrated model of eicosanoid metabolism and signaling based on lipidomics flux analysis.Gupta S, Maurya MR, Stephens DL, Dennis EA, Subramaniam S.Biophys. J. 2009 Jun; 96(11):4542-51.

Abstract:

There is increasing evidence for a major and critical involvement of lipids in signal transduction and cellular trafficking, and this has motivated large-scale studies on lipid pathways. The Lipid Metabolites and Pathways Strategy consortium is actively investigating lipid metabolism in mammalian cells and has made available time-course data on various lipids in response to treatment with KDO(2)-lipid A (a lipopolysaccharide analog) of macrophage RAW 264.7 cells. The lipids known as eicosanoids play an important role in inflammation. We have reconstructed an integrated network of eicosanoid metabolism and signaling based on the KEGG pathway database and the literature and have developed a kinetic model. A matrix-based approach was used to estimate the rate constants from experimental data and these were further refined using generalized constrained nonlinear optimization. The resulting model fits the experimental data well for all species, and simulated enzyme activities were similar to their literature values. The quantitative model for eicosanoid metabolism that we have developed can be used to design experimental studies utilizing genetic and pharmacological perturbations to probe fluxes in lipid pathways.

This model is hosted on BioModels Database and identified by: BIOMD0000000436 .

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

2 Unit Definitions

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

2.1 Unit `time`

Definition 3600 s

2.2 Unit `perh`

Definition $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$

2.3 Unit pmolperugDNA

Definition $\mathrm{pmol} \cdot \mu\mathrm{g}^{-1}$

2.4 Unit ug

Definition $\mu\mathrm{g}$

2.5 Unit pmol

Definition pmol

2.6 Unit pmolperh

Definition $\mathrm{pmol} \cdot \left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$

2.7 Unit ugDNAperh

Definition $\mu\mathrm{g} \cdot \left(3600\ \mathrm{s}\right)^{-1}$

2.8 Unit substance

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

2.9 Unit volume

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.10 Unit area

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

Definition m^2

2.11 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
c1			3	1		☑	

3.1 Compartment c1

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

4 Species

This model contains 13 species. The boundary condition of one of these species is set to `true` so that this species' amount cannot be changed by any reaction. Section 10 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
FA		c1	pmol	☑	☑
HETE		c1	pmol	☐	☐
PGH2		c1	pmol	☐	☐
PGE2		c1	pmol	☐	☐
PGF2a		c1	pmol	☐	☐
PGD2		c1	mol	☐	☐
PGJ2		c1	pmol	☐	☐
dPGJ2		c1	pmol	☐	☐
AA	Arachidonic acid	c1	pmol	☐	☐
LPS		c1	dimensionless $\cdot\, l^{-1}$	☐	☐
DG		c1	dimensionless $\cdot\, l^{-1}$	☐	☐
GPCho		c1	pmol	☐	☐
dPGD2		c1	pmol	☐	☐

5 Parameters

This model contains 77 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1		0000009	355.637	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k2		0000009	10^{-15}	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k3		0000009	10^{-15}	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k4		0000009	10^{-15}	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k5		0000009	10^{-15}	$\mu\mathrm{g} \cdot (3600\ \mathrm{s})^{-1}$	☑
k6		0000009	0.330	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k7		0000009	10^{-15}	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k8		0000009	0.007	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k9		0000009	0.187	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k10		0000009	0.024	$\mu\mathrm{g} \cdot (3600\ \mathrm{s})^{-1}$	☑
k11		0000009	0.111	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k12		0000009	0.098	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k13		0000009	0.204	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k14		0000009	10^{-15}	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k15		0000009	0.061	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k16		0000009	10^{-15}	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k17		0000009	3.116	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k18		0000009	0.054	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k19		0000009	0.029	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k20		0000009	0.014	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k21		0000009	0.034	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
k22		0000009	0.116	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
DNA		0000002	1.000	$\mu\mathrm{g}$	☑
DGperDNA		0000002	1.000	$\mathrm{pmol} \cdot \mu\mathrm{g}^{-1}$	⊟
onepmol			1.000	pmol	☑
t0			0.000	3600 s	☑
t1			0.500	3600 s	☑
t2			1.000	3600 s	☑
t3			2.000	3600 s	☑
t4			4.000	3600 s	☑
t5			8.000	3600 s	☑
t6			12.000	3600 s	☑
timevalue			0.000	3600 s	⊟

Id	Name	SBO	Value	Unit	Constant
zero			0.000	dimensionless	☑
LPSactivity			0.000	dimensionless	⊟
LPSslope			0.000	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	⊟
LPSint			0.000	dimensionless	⊟
LPSslopezero			2.000	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
LPSslope1			−0.667	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
LPSslope3			0.000	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
LPSintzero			0.000	dimensionless	☑
LPSint1			1.334	dimensionless	☑
LPSint3			0.000	dimensionless	☑
DGactivity			1.000	dimensionless	⊟
DGint			1.000	dimensionless	⊟
DGslope			1.000	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	⊟
DGslopezero			0.301	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
DGslope1			−0.157	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
DGslope2			0.044	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
DGslope3			−0.091	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
DGslope4			0.098	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
DGslope5			0.071	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
DGslope6			0.085	$\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
DGintzero			1.000	dimensionless	☑
DGint1			1.229	dimensionless	☑
DGint2			1.028	dimensionless	☑
DGint3			1.299	dimensionless	☑
DGint4			0.543	dimensionless	☑
DGint5			0.755	dimensionless	☑
DGint6			0.593	dimensionless	☑
GPChoratio			1.000	dimensionless	⊟
GPChoint			315.314	pmol	⊟
GPChoslope			−158.430	pmol · $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	⊟
GPChoslopezero			−158.430	pmol · $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
GPChoslope1			112.280	pmol · $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
GPChoslope2			24.310	pmol · $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
GPChoslope3			−39.930	pmol · $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
GPChoslope4			5.480	pmol $\cdot$ $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
GPChoslope5			27.080	pmol $\cdot$ $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
GPChoslope6			−4.874	pmol $\cdot$ $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1}$	☑
GPChointzero			315.314	pmol	☑
GPChoint1			179.960	pmol	☑
GPChoint2			267.930	pmol	☑
GPChoint3			396.410	pmol	☑
GPChoint4			214.770	pmol	☑
GPChoint5			41.930	pmol	☑
GPChoint6			425.430	pmol	☑

6 Function definition

This is an overview of one function definition.

6.1 Function definition activitycalc

Arguments x, slopea, yintercepta

Mathematical Expression

$$\mathrm{yintercepta} + \mathrm{x} \cdot \mathrm{slopea} \tag{1}$$

7 Rules

This is an overview of four rules.

7.1 Rule timevalue

Rule timevalue is an assignment rule for parameter timevalue:

$$\mathrm{timevalue} = \mathrm{t} + \mathrm{t0} \tag{2}$$

Derived unit 3600 s

7.2 Rule LPSactivity

Rule LPSactivity is an assignment rule for parameter LPSactivity:

$$\mathrm{LPSactivity} = \mathrm{activitycalc}\left(\mathrm{timevalue}, \mathrm{LPSslope}, \mathrm{LPSint}\right) \tag{3}$$

Derived unit dimensionless

7.3 Rule DGactivity

Rule DGactivity is an assignment rule for parameter DGactivity:

$$\text{DGactivity} = \text{activitycalc}\left(\text{timevalue}, \text{DGslope}, \text{DGint}\right) \tag{4}$$

Derived unit dimensionless

7.4 Rule GPChoratio

Rule GPChoratio is an assignment rule for parameter GPChoratio:

$$\text{GPChoratio} = \frac{\text{activitycalc}\left(\text{timevalue}, \text{GPChoslope}, \text{GPChoint}\right)}{\text{GPChointzero}} \tag{5}$$

Derived unit dimensionless

8 Events

This is an overview of seven events. Each event is initiated whenever its trigger condition switches from false to true. A delay function postpones the effects of an event to a later time point. At the time of execution, an event can assign values to species, parameters or compartments if these are not set to constant.

8.1 Event event_0

Trigger condition

$$\text{timevalue} > \text{t0} \tag{6}$$

Assignments

$$\text{LPSint} = \text{LPSintzero} \tag{7}$$
$$\text{LPSslope} = \text{LPSslopezero} \tag{8}$$
$$\text{DGint} = \text{DGintzero} \tag{9}$$
$$\text{DGslope} = \text{DGslopezero} \tag{10}$$
$$\text{GPChoint} = \text{GPChointzero} \tag{11}$$
$$\text{GPChoslope} = \text{GPChoslopezero} \tag{12}$$

8.2 Event event_1

Trigger condition

$$\text{timevalue} \geq \text{t1} \tag{13}$$

Assignments

$$\text{LPSint} = \text{LPSint1} \tag{14}$$
$$\text{LPSslope} = \text{LPSslope1} \tag{15}$$
$$\text{DGint} = \text{DGint1} \tag{16}$$
$$\text{DGslope} = \text{DGslope1} \tag{17}$$
$$\text{GPChoint} = \text{GPChoint1} \tag{18}$$
$$\text{GPChoslope} = \text{GPChoslope1} \tag{19}$$

8.3 Event event_2

Trigger condition

$$\text{timevalue} \geq \text{t2} \tag{20}$$

Assignments

$$\text{DGint} = \text{DGint2} \tag{21}$$
$$\text{DGslope} = \text{DGslope2} \tag{22}$$
$$\text{GPChoint} = \text{GPChoint2} \tag{23}$$
$$\text{GPChoslope} = \text{GPChoslope2} \tag{24}$$

8.4 Event event_3

Trigger condition

$$\text{timevalue} \geq \text{t3} \tag{25}$$

Assignments

$$\text{LPSint} = \text{LPSint3} \tag{26}$$
$$\text{LPSslope} = \text{LPSslope3} \tag{27}$$
$$\text{DGint} = \text{DGint3} \tag{28}$$
$$\text{DGslope} = \text{DGslope3} \tag{29}$$
$$\text{GPChoint} = \text{GPChoint3} \tag{30}$$
$$\text{GPChoslope} = \text{GPChoslope3} \tag{31}$$

8.5 Event event_4

Trigger condition

$$\text{timevalue} \geq \text{t4} \tag{32}$$

Assignments

$$\text{DGint} = \text{DGint4} \tag{33}$$
$$\text{DGslope} = \text{DGslope4} \tag{34}$$
$$\text{GPChoint} = \text{GPChoint4} \tag{35}$$
$$\text{GPChoslope} = \text{GPChoslope4} \tag{36}$$

8.6 Event event_5

Trigger condition

$$\text{timevalue} \geq \text{t5} \tag{37}$$

Assignments

$$\text{DGint} = \text{DGint5} \tag{38}$$
$$\text{DGslope} = \text{DGslope5} \tag{39}$$
$$\text{GPChoint} = \text{GPChoint5} \tag{40}$$
$$\text{GPChoslope} = \text{GPChoslope5} \tag{41}$$

8.7 Event event_6

Trigger condition

$$\text{timevalue} \geq \text{t6} \tag{42}$$

Assignments

$$\text{DGint} = \text{DGint6} \tag{43}$$
$$\text{DGslope} = \text{DGslope6} \tag{44}$$
$$\text{GPChoint} = \text{GPChoint6} \tag{45}$$
$$\text{GPChoslope} = \text{GPChoslope6} \tag{46}$$

9 Reactions

This model contains 22 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	r2		FA $\longrightarrow$ AA	
2	r3		DG $\longrightarrow$ AA	
3	r7		GPCho $\longrightarrow$ AA	
4	r5		GPCho $\xrightarrow{\text{DG}}$ AA	
5	r11		AA $\xrightarrow{\text{LPS}}$ PGH2	
6	r10		AA $\xrightarrow{\text{DG}}$ PGH2	
7	r8		AA $\longrightarrow$ HETE	
8	r4		AA $\longrightarrow \emptyset$	
9	r9		HETE $\longrightarrow \emptyset$	
10	r13		PGH2 $\longrightarrow$ PGE2	
11	r14		PGE2 $\longrightarrow \emptyset$	
12	r15		PGH2 $\longrightarrow$ PGF2a	
13	r16		PGF2a $\longrightarrow \emptyset$	
14	r17		PGH2 $\longrightarrow$ PGD2	
15	r18		PGD2 $\longrightarrow$ PGJ2	
16	r19		PGD2 $\longrightarrow$ dPGD2	
17	r20		dPGD2 $\longrightarrow \emptyset$	
18	r21		PGJ2 $\longrightarrow$ dPGJ2	
19	r22		dPGJ2 $\longrightarrow \emptyset$	
20	r1		FA $\xrightarrow{\text{LPS}}$ AA	
21	r6		GPCho $\xrightarrow{\text{LPS}}$ AA	

№	Id	Name	Reaction Equation	SBO
22	r12		AA ⟶ PGH2	

9.1 Reaction r2

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

Reaction equation

$$\mathrm{FA} \longrightarrow \mathrm{AA} \tag{47}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
FA		

Product

Table 7: Properties of each product.

Id	Name	SBO
AA	Arachidonic acid	

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_1 = \mathrm{k2} \cdot \mathrm{FA} \tag{48}$$

9.2 Reaction r3

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

Reaction equation

$$\mathrm{DG} \longrightarrow \mathrm{AA} \tag{49}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
DG		

Product

Table 9: Properties of each product.

Id	Name	SBO
AA	Arachidonic acid	

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_2 = \mathrm{k3} \cdot \mathrm{DGactivity} \cdot \mathrm{DGperDNA} \cdot \mathrm{DNA} \tag{50}$$

9.3 Reaction r7

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

Reaction equation

$$\mathrm{GPCho} \longrightarrow \mathrm{AA} \tag{51}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
GPCho		

Product

Table 11: Properties of each product.

Id	Name	SBO
AA	Arachidonic acid	

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_3 = \mathrm{k7} \cdot \mathrm{GPChoratio} \cdot \mathrm{GPCho} \tag{52}$$

9.4 Reaction r5

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

Reaction equation

$$\text{GPCho} \xrightarrow{\text{DG}} \text{AA} \tag{53}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
GPCho		

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
DG		

Product

Table 14: Properties of each product.

Id	Name	SBO
AA	Arachidonic acid	

Kinetic Law

Derived unit $(3600\ \text{s})^{-1} \cdot \text{pmol}$

$$v_4 = \frac{\text{k5} \cdot \text{DGactivity} \cdot \text{GPChoratio} \cdot \text{GPCho}}{\text{DNA}} \tag{54}$$

9.5 Reaction r11

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

Reaction equation

$$\text{AA} \xrightarrow{\text{LPS}} \text{PGH2} \tag{55}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
AA	Arachidonic acid	

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
LPS		

Product

Table 17: Properties of each product.

Id	Name	SBO
PGH2		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_5 = \mathrm{k11} \cdot \mathrm{AA} \tag{56}$$

9.6 Reaction r10

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

Reaction equation

$$\mathrm{AA} \xrightarrow{\mathrm{DG}} \mathrm{PGH2} \tag{57}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
AA	Arachidonic acid	

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
DG		

Product

Table 20: Properties of each product.

Id	Name	SBO
PGH2		

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{pmol}$

$$v_6 = \frac{\mathrm{k10} \cdot \mathrm{DGactivity} \cdot \mathrm{AA}}{\mathrm{DNA}} \tag{58}$$

9.7 Reaction r8

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

Reaction equation

$$\mathrm{AA} \longrightarrow \mathrm{HETE} \tag{59}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
AA	Arachidonic acid	

Product

Table 22: Properties of each product.

Id	Name	SBO
HETE		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_7 = \mathrm{k8} \cdot \mathrm{AA} \tag{60}$$

9.8 Reaction r4

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

Reaction equation

$$\mathrm{AA} \longrightarrow \emptyset \tag{61}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
AA	Arachidonic acid	

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_8 = \mathrm{k4} \cdot \mathrm{AA} \tag{62}$$

9.9 Reaction r9

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

Reaction equation

$$\mathrm{HETE} \longrightarrow \emptyset \tag{63}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
HETE		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_9 = \mathrm{k9} \cdot \mathrm{HETE} \tag{64}$$

9.10 Reaction r13

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

Reaction equation

$$\mathrm{PGH2} \longrightarrow \mathrm{PGE2} \tag{65}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
PGH2		

Product

Table 26: Properties of each product.

Id	Name	SBO
PGE2		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_{10} = \mathrm{k13} \cdot \mathrm{PGH2} \tag{66}$$

9.11 Reaction r14

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

Reaction equation

$$\mathrm{PGE2} \longrightarrow \emptyset \tag{67}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
PGE2		

Kinetic Law

SBO:0000044 mass action rate law for first order irreversible reactions

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_{11} = \mathrm{k14} \cdot \mathrm{PGE2} \tag{68}$$

9.12 Reaction r15

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

Reaction equation

$$\mathrm{PGH2} \longrightarrow \mathrm{PGF2a} \tag{69}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
PGH2		

Product

Table 29: Properties of each product.

Id	Name	SBO
PGF2a		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_{12} = \mathrm{k15} \cdot \mathrm{PGH2} \tag{70}$$

9.13 Reaction r16

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

Reaction equation

$$\mathrm{PGF2a} \longrightarrow \emptyset \tag{71}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
PGF2a		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_{13} = \mathrm{k16} \cdot \mathrm{PGF2a} \tag{72}$$

9.14 Reaction r17

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

Reaction equation

$$\mathrm{PGH2} \longrightarrow \mathrm{PGD2} \tag{73}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
PGH2		

Product

Table 32: Properties of each product.

Id	Name	SBO
PGD2		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_{14} = \mathrm{k17} \cdot \mathrm{PGH2} \tag{74}$$

9.15 Reaction r18

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

Reaction equation

$$\mathrm{PGD2} \longrightarrow \mathrm{PGJ2} \tag{75}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
PGD2		

Product

Table 34: Properties of each product.

Id	Name	SBO
PGJ2		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{mol}$

$$v_{15} = \mathrm{k18} \cdot \mathrm{PGD2} \tag{76}$$

9.16 Reaction r19

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

Reaction equation

$$\mathrm{PGD2} \longrightarrow \mathrm{dPGD2} \tag{77}$$

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
PGD2		

Product

Table 36: Properties of each product.

Id	Name	SBO
dPGD2		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{mol}$

$$v_{16} = \mathrm{k19} \cdot \mathrm{PGD2} \tag{78}$$

9.17 Reaction r20

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

Reaction equation

$$\mathrm{dPGD2} \longrightarrow \emptyset \tag{79}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
dPGD2		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_{17} = \mathrm{k20} \cdot \mathrm{dPGD2} \tag{80}$$

9.18 Reaction r21

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

Reaction equation

$$\mathrm{PGJ2} \longrightarrow \mathrm{dPGJ2} \tag{81}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
PGJ2		

Product

Table 39: Properties of each product.

Id	Name	SBO
dPGJ2		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_{18} = \mathrm{k21} \cdot \mathrm{PGJ2} \tag{82}$$

9.19 Reaction r22

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

Reaction equation

$$\mathrm{dPGJ2} \longrightarrow \emptyset \tag{83}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
dPGJ2		

Kinetic Law

SBO:0000001 rate law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_{19} = \mathrm{k22} \cdot \mathrm{dPGJ2} \tag{84}$$

9.20 Reaction r1

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

Reaction equation

$$\mathrm{FA} \xrightarrow{\mathrm{LPS}} \mathrm{AA} \tag{85}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
FA		

Modifier

Table 42: Properties of each modifier.

Id	Name	SBO
LPS		

Product

Table 43: Properties of each product.

Id	Name	SBO
AA	Arachidonic acid	

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_{20} = \mathrm{k1} \cdot \mathrm{onepmol} \cdot \mathrm{LPSactivity} \tag{86}$$

9.21 Reaction `r6`

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

Reaction equation

$$\mathrm{GPCho} \xrightarrow{\mathrm{LPS}} \mathrm{AA} \tag{87}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
`GPCho`		

Modifier

Table 45: Properties of each modifier.

Id	Name	SBO
`LPS`		

Product

Table 46: Properties of each product.

Id	Name	SBO
`AA`	Arachidonic acid	

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_{21} = \mathrm{k6} \cdot \mathrm{GPCho} \cdot \mathrm{GPChoratio} \cdot \mathrm{LPSactivity} \tag{88}$$

9.22 Reaction r12

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

Reaction equation

$$\mathrm{AA} \longrightarrow \mathrm{PGH2} \tag{89}$$

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
AA	Arachidonic acid	

Product

Table 48: Properties of each product.

Id	Name	SBO
PGH2		

Kinetic Law

Derived unit $\left(2.778 \cdot 10^{-4}\ \mathrm{s}\right)^{-1} \cdot \mathrm{pmol}$

$$v_{22} = \mathrm{k12} \cdot \mathrm{AA} \cdot \mathrm{LPSactivity} \tag{90}$$

10 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.

10.1 Species FA

Notes Fatty acyls

Initial amount 1 *Unknownunit pmol*

This species takes part in two reactions (as a reactant in r2, r1), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FA} = 0 \tag{91}$$

10.2 Species HETE

Initial amount 0 *Unknownunit pmol*

This species takes part in two reactions (as a reactant in r9 and as a product in r8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{HETE} = v_7 - v_9 \tag{92}$$

10.3 Species PGH2

Initial amount 0 *Unknownunit pmol*

This species takes part in six reactions (as a reactant in r13, r15, r17 and as a product in r11, r10, r12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PGH2} = v_5 + v_6 + v_{22} - v_{10} - v_{12} - v_{14} \tag{93}$$

10.4 Species PGE2

Initial amount 0 *Unknownunit pmol*

This species takes part in two reactions (as a reactant in r14 and as a product in r13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PGE2} = v_{10} - v_{11} \tag{94}$$

10.5 Species PGF2a

Initial amount 0 *Unknownunit pmol*

This species takes part in two reactions (as a reactant in r16 and as a product in r15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PGF2a} = v_{12} - v_{13} \tag{95}$$

10.6 Species PGD2

Initial amount 0 mol

This species takes part in three reactions (as a reactant in r18, r19 and as a product in r17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PGD2} = v_{14} - v_{15} - v_{16} \tag{96}$$

10.7 Species PGJ2

Initial amount 0 *Unknownunit pmol*

This species takes part in two reactions (as a reactant in r21 and as a product in r18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PGJ2} = v_{15} - v_{18} \tag{97}$$

10.8 Species dPGJ2

Initial amount 0 *Unknownunit pmol*

This species takes part in two reactions (as a reactant in r22 and as a product in r21).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{dPGJ2} = v_{18} - v_{19} \tag{98}$$

10.9 Species AA

Name Arachidonic acid

Initial amount 25 *Unknownunit pmol*

This species takes part in eleven reactions (as a reactant in r11, r10, r8, r4, r12 and as a product in r2, r3, r7, r5, r1, r6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AA} = v_1 + v_2 + v_3 + v_4 + v_{20} + v_{21} - v_5 - v_6 - v_7 - v_8 - v_{22} \tag{99}$$

10.10 Species LPS

Initial amount 0.5 dimensionless

This species takes part in three reactions (as a modifier in r11, r1, r6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{LPS} = 0 \tag{100}$$

10.11 Species DG

Notes Arachidonic acid-containing glycerophospholipids

Initial amount 0 dimensionless

This species takes part in three reactions (as a reactant in r3 and as a modifier in r5, r10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DG} = -v_2 \tag{101}$$

10.12 Species GPCho

Notes Glycerophosphocholines

Initial amount 1 *Unknownunit pmol*

This species takes part in three reactions (as a reactant in r7, r5, r6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GPCho} = -v_3 - v_4 - v_{21} \tag{102}$$

10.13 Species dPGD2

Initial amount 0 *Unknownunit pmol*

This species takes part in two reactions (as a reactant in r20 and as a product in r19).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{dPGD2} = v_{16} - v_{17} \tag{103}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000001 rate law: mathematical description that relates quantities of reactants to the reaction velocity

SBO:0000002 quantitative systems description parameter: A numerical value that defines certain characteristics of systems or system functions. It may be part of a calculation, but its value is not determined by the form of the equation itself, and may be arbitrarily assigned

SBO:0000009 kinetic constant: Numerical parameter that quantifies the velocity of a chemical reaction

SBO:0000044 mass action rate law for first order irreversible reactions: 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

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