SBML Model Report

Model name: “Kolodkin2013 - Nuclear receptor-mediated cortisol signalling network”

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Alastair Hume[1] and Nilgun Sahin[2] at July third 2015 at 11:56 a. m. and last time modified at September nineth 2015 at 11:03 a. m. Table 1 gives 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	2
species types	0	species	42
events	0	constraints	0
reactions	52	function definitions	3
global parameters	11	unit definitions	2
rules	2	initial assignments	0

Model Notes

Kolodkin2013 - Nuclear receptor-mediatedcortisol signalling network

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This model is described in the article:Optimization of stress response through the nuclear receptor-mediated cortisol signalling network.Kolodkin A, Sahin N, Phillips A, Hood SR, Bruggeman FJ, Westerhoff HV, Plant N.Nat Commun 2013; 4: 1792

Abstract:

It is an accepted paradigm that extended stress predisposes an individual to pathophysiology. However, the biological adaptations to minimize this risk are poorly understood. Using a computational model based upon realistic kinetic parameters we are able to reproduce the interaction of the stress hormone cortisol with its two nuclear receptors, the high-affinity glucocorticoid receptor and the low-affinity pregnane X-receptor. We demonstrate that regulatory signals between these two nuclear receptors are necessary to optimize the body's response to stress episodes, attenuating both the magnitude and duration of the biological response. In addition, we predict that the activation of pregnane X-receptor by multiple, low-affinity endobiotic ligands is necessary for the significant pregnane X-receptor-mediated transcriptional response observed following stress episodes. This integration allows responses mediated through both the high and low-affinity nuclear receptors, which we predict is an important strategy to minimize the risk of disease from chronic stress.

This model is hosted on BioModels Database and identified by: BIOMD0000000576.

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

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 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
default	default		3	1	litre	☑	
blood	blood		3	5	l	☑	

3.1 Compartment default

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

Name default

3.2 Compartment blood

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

Name blood

4 Species

This model contains 42 species. The boundary condition of eight of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 9 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
s28	S_RNA	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑
s36	S_PROT	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑
s46	PXR_GENE	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s32	PXR_RNA	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s42	PXR_PROT	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s30	P	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑
s40	GR_GENE	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s33	GR_RNA	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s39	GR_PROT	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s114	Cort	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s155	CYP_GENE	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s172	CYP_PROT	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s173	CYP_RNA	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s185	TAT_RNA	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s84	GRgene_GRprot_Cort	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s165	CYPgene_PXRprot_Cort	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s109	PXRgene_GRprot_Cort	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s87	GRprot_Cort	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s119	PXRprot_Cort	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s183	TATgene_GRprot_Cort	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
s178	TAT_GENE	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
s10	Cort_degr	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑
Cortisone	Cortisone	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑
TAT_PROT	TAT_PROT	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Ligand2	Ligand2	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PXRprot_Ligand2	PXRprot_Ligand2	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CYPgene_PXRprot_Ligand2	CYPgene_PXRprot_Ligand2	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DEX	DEX	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GRprot_DEX	GRprot_DEX	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PXRprot_DEX	PXRprot_DEX	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DEX_degr	DEX_degr	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑
CYPgene_PXRprot_DEX	CYPgene_PXRprot_DEX	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PXRgene_GRprot_DEX	PXRgene_GRprot_DEX	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GRgene_GRprot_DEX	GRgene_GRprot_DEX	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
TATgene_GRprot_DEX	TATgene_GRprot_DEX	default	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
s2	CortOUT	blood	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DEXout	DEXout	blood	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑
CBG	CBG	blood	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CBG_CortOUT	CBG_CortOUT	blood	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Alb	Alb	blood	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Alb_CortOUT	Alb_CortOUT	blood	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CortAdded	CortAdded	blood	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑

5 Parameters

This model contains eleven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
GeneProteinBinding_diff_limited	GeneProteinBinding_diff_limited		60.000		☑
cypGene_PXRprotein	cypGene_PXRprotein		1.000		☑
cypMrna_synt	cypMrna_synt		0.050		☑
PXRGene_GRprotein	PXRGene_GRprotein		200.000		☑
TATGene_GRprotein	TATGene_GRprotein		300.000		☑
GRGene_GRprotein	GRGene_GRprotein		60.000		☑
grMrna_synt	grMrna_synt		$1.2 \cdot 10^{-6}$		☑
tatMrna_synt	tatMrna_synt		0.005		☑
pxrMrna_synt	pxrMrna_synt		$1.1 \cdot 10^{-4}$		☑
GRprotein	GRprotein		80.000		⊟
PXRprotein	PXRprotein		99.911		⊟

6 Function definitions

This is an overview of three function definitions.

6.1 Function definition mRNA

Name mRNA

Arguments S_RNA, Activator, Ka

Mathematical Expression

$$\mathrm{Ka} \cdot \mathrm{S\_RNA} \cdot \mathrm{Activator} \tag{1}$$

6.2 Function definition ptotein

Name ptotein

Arguments Ka, S_PROT, Activator

Mathematical Expression

$$\mathrm{Ka} \cdot \mathrm{S\_PROT} \cdot \mathrm{Activator} \tag{2}$$

6.3 Function definition LigandDegrOld

Name LigandDegrOld

Arguments Act, Vm, S1, Kms1, S2, Kms2, S3, Kms3

Mathematical Expression

$$\text{Act} \cdot \frac{\frac{\text{Vm} \cdot \text{S1}}{\text{Kms1}}}{1 + \frac{\text{S1}}{\text{Kms1}} + \frac{\text{S2}}{\text{Kms2}} + \frac{\text{S3}}{\text{Kms3}}} \tag{3}$$

7 Rules

This is an overview of two rules.

7.1 Rule GRprotein

Rule GRprotein is an assignment rule for parameter GRprotein:

$$\begin{aligned}\text{GRprotein} = {} & [\text{s39}] + [\text{s84}] + [\text{s109}] + [\text{s87}] + [\text{s183}] + [\text{GRprot\_DEX}] \\ & + [\text{PXRgene\_GRprot\_DEX}] + [\text{GRgene\_GRprot\_DEX}] + [\text{TATgene\_GRprot\_DEX}]\end{aligned} \tag{4}$$

Derived unit $\text{nmol} \cdot \text{l}^{-1}$

7.2 Rule PXRprotein

Rule PXRprotein is an assignment rule for parameter PXRprotein:

$$\begin{aligned}\text{PXRprotein} = {} & [\text{s42}] + [\text{s165}] + [\text{s119}] + [\text{PXRprot\_Ligand2}] + [\text{CYPgene\_PXRprot\_Ligand2}] \\ & + [\text{PXRprot\_DEX}] + [\text{CYPgene\_PXRprot\_DEX}]\end{aligned} \tag{5}$$

Derived unit $\text{nmol} \cdot \text{l}^{-1}$

8 Reactions

This model contains 52 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	re1	re1	$s28 \xrightarrow{s155,\ s28,\ s155} s173$	
2	re2	re2	$s173 \xrightarrow{s173} s30$	
3	re3	re3	$s36 \xrightarrow{s173,\ s36,\ s173} s172$	
4	re4	re4	$s172 \xrightarrow{s172} s30$	
5	re5	re5	$s28 \xrightarrow{s46,\ s28,\ s46} s32$	
6	re6	re6	$s32 \xrightarrow{s32} s30$	
7	re7	re7	$s36 \xrightarrow{s32,\ s36,\ s32} s42$	
8	re8	re8	$s42 \xrightarrow{s42} s30$	
9	re9	re9	$s28 \xrightarrow{s40,\ s28,\ s40} s33$	
10	re10	re10	$s33 \xrightarrow{s33} s30$	
11	re11	re11	$s36 \xrightarrow{s33,\ s36,\ s33} s39$	
12	re12	re12	$s39 \xrightarrow{s39} s30$	
13	re13	re13	$s28 \xrightarrow{s178,\ s28,\ s178} s185$	
14	re14	re14	$s185 \xrightarrow{s185} s30$	
15	re15	re15	$s114 + s39 \xrightleftharpoons{s114,\ s39,\ s87} s87$	
16	re16	re16	$s87 \xrightarrow{s87} s114 + s30$	

№	Id	Name	Reaction Equation	SBO
17	re17	re17	$s42 + s114 \overset{s42,\ s114,\ s119}{\rightleftharpoons} s119$	
18	re18	re18	$s119 \overset{s119}{\longrightarrow} s114 + s30$	
19	re19	re19	$s114 \overset{s172,\ Ligand2,\ DEX,\ s172,\ s114,\ Ligand2,\ DEX}{\longrightarrow} s10$	
20	re20	re20	$s155 + s119 \overset{s155,\ s119,\ s165}{\rightleftharpoons} s165$	
21	re21	re21	$s28 \overset{s165,\ s28,\ s165}{\longrightarrow} s173$	
22	re22	re22	$s46 + s87 \overset{s46,\ s87,\ s109}{\rightleftharpoons} s109$	
23	re23	re23	$s28 \overset{s109,\ s28,\ s109}{\longrightarrow} s32$	
24	re24	re24	$s40 + s87 \overset{s40,\ s87,\ s84}{\rightleftharpoons} s84$	
25	re25	re25	$s28 \overset{s84,\ s28,\ s84}{\longrightarrow} s33$	
26	re26	re26	$s178 + s87 \overset{s178,\ s87,\ s183}{\rightleftharpoons} s183$	
27	re27	re27	$s28 \overset{s183,\ s28,\ s183}{\longrightarrow} s185$	
28	re42	re42	$Cortisone \overset{Cortisone,\ s114}{\rightleftharpoons} s114$	
29	re44	re44	$TAT\_PROT \overset{TAT\_PROT}{\longrightarrow} s30$	
30	re43	re43	$s36 \overset{s185,\ s36,\ s185}{\longrightarrow} TAT\_PROT$	
31	cortisolTransport	cortisolTransport	$s2 \overset{s2,\ s114}{\rightleftharpoons} s114$	
32	L2_PXR_binding	L2_PXR_binding	$s42 + Ligand2 \overset{s42,\ Ligand2,\ PXRprot\_Ligand2}{\rightleftharpoons} PXRprot\_Ligand2$	
33	L2_PXR_deg	L2_PXR_deg	$PXRprot\_Ligand2 \overset{PXRprot\_Ligand2}{\longrightarrow} Ligand2 + s30$	
34	CYPmRNA_synt_PXR_L2	CYPmRNA_synt_PXR_L2	$s28 \overset{CYPgene\_PXRprot\_Ligand2,\ s28,\ CYPgene\_PXRprot\_Ligand2}{\longrightarrow} s173$	

№	Id	Name	Reaction Equation	SBO
35	CYPmRNA_PXR_L2_binding	CYPmRNA_PXR_L2_binding	$s155 + PXRprot\_Ligand2 \overset{s155,\ PXRprot\_Ligand2,\ CYPgene\_PXRprot\_Ligand2}{\rightleftharpoons} CYPg$	
36	re28	re28	$s39 + DEX \overset{s39,\ DEX,\ GRprot\_DEX}{\rightleftharpoons} GRprot\_DEX$	
37	re29	re29	$GRprot\_DEX \xrightarrow{GRprot\_DEX} s30 + DEX$	
38	re30	re30	$s42 + DEX \overset{s42,\ DEX,\ PXRprot\_DEX}{\rightleftharpoons} PXRprot\_DEX$	
39	re31	re31	$PXRprot\_DEX \xrightarrow{PXRprot\_DEX} DEX + s30$	
40	re32	re32	$DEX \xrightarrow{s172,\ Ligand2,\ s114,\ s172,\ DEX,\ Ligand2,\ s114} DEX\_degr$	
41	re33	re33	$s155 + PXRprot\_DEX \overset{s155,\ PXRprot\_DEX,\ CYPgene\_PXRprot\_DEX}{\rightleftharpoons} CYPgene\_PXR$	
42	re34	re34	$s28 \xrightarrow{CYPgene\_PXRprot\_DEX,\ s28,\ CYPgene\_PXRprot\_DEX} s173$	
43	re35	re35	$GRprot\_DEX + s46 \overset{GRprot\_DEX,\ s46,\ PXRgene\_GRprot\_DEX}{\rightleftharpoons} PXRgene\_GRprot\_DE$	
44	re36	re36	$s28 \xrightarrow{PXRgene\_GRprot\_DEX,\ s28,\ PXRgene\_GRprot\_DEX} s32$	
45	re37	re37	$GRprot\_DEX + s40 \overset{GRprot\_DEX,\ s40,\ GRgene\_GRprot\_DEX}{\rightleftharpoons} GRgene\_GRprot\_DEX$	
46	re38	re38	$s28 \xrightarrow{GRgene\_GRprot\_DEX,\ s28,\ GRgene\_GRprot\_DEX} s33$	
47	re39	re39	$GRprot\_DEX + s178 \overset{GRprot\_DEX,\ s178,\ TATgene\_GRprot\_DEX}{\rightleftharpoons} TATgene\_GRprot\_D$	
48	re40	re40	$s28 \xrightarrow{TATgene\_GRprot\_DEX,\ s28,\ TATgene\_GRprot\_DEX} s185$	
49	re41	re41	$DEXout \overset{DEXout,\ DEX}{\rightleftharpoons} DEX$	
50	Cortisol_CBG	Cortisol_CBG	$s2 + CBG \overset{s2,\ CBG,\ CBG\_CortOUT}{\rightleftharpoons} CBG\_CortOUT$	
51	Cort_Alb	Cort_Alb	$Alb + s2 \overset{Alb,\ s2,\ Alb\_CortOUT}{\rightleftharpoons} Alb\_CortOUT$	
52	cort_distribution	cort_distribution	$CortAdded \xrightarrow{CortAdded} s2$	

№	Id	Name	Reaction Equation	SBO

8.1 Reaction re1

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

Name re1

Reaction equation

$$\text{s28} \xrightarrow{\text{s155, s28, s155}} \text{s173} \tag{6}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
s155	CYP_GENE	
s28	S_RNA	
s155	CYP_GENE	

Product

Table 8: Properties of each product.

Id	Name	SBO
s173	CYP_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\,(\text{default}) \cdot \text{mRNA}\,([\text{s28}], [\text{s155}], \text{Ka}) \tag{7}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{8}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{9}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ka	Ka		0.003		☑

8.2 Reaction re2

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

Name re2

Reaction equation

$$\mathrm{s173} \xrightarrow{\mathrm{s173}} \mathrm{s30} \tag{10}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
s173	CYP_RNA	

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
s173	CYP_RNA	

Product

Table 12: Properties of each product.

Id	Name	SBO
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k1} \cdot [\mathrm{s173}] \tag{11}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.04		☑

8.3 Reaction re3

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

Name re3

Reaction equation

$$\text{s36} \xrightarrow{\text{s173, s36, s173}} \text{s172} \tag{12}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
s36	S_PROT	

Modifiers

Table 15: Properties of each modifier.

Id	Name	SBO
s173	CYP_RNA	
s36	S_PROT	
s173	CYP_RNA	

Product

Table 16: Properties of each product.

Id	Name	SBO
s172	CYP_PROT	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{ptotein}\,(\mathrm{Ka}, [\mathrm{s36}], [\mathrm{s173}]) \tag{13}$$

$$\mathrm{ptotein}\,(\mathrm{Ka}, \mathrm{S\_PROT}, \mathrm{Activator}) = \mathrm{Ka} \cdot \mathrm{S\_PROT} \cdot \mathrm{Activator} \tag{14}$$

$$\mathrm{ptotein}\,(\mathrm{Ka}, \mathrm{S\_PROT}, \mathrm{Activator}) = \mathrm{Ka} \cdot \mathrm{S\_PROT} \cdot \mathrm{Activator} \tag{15}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ka	Ka		2.5		☑

8.4 Reaction re4

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

Name re4

Reaction equation

$$\mathrm{s172} \xrightarrow{\mathrm{s172}} \mathrm{s30} \tag{16}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
s172	CYP_PROT	

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
s172	CYP_PROT	

Product

Table 20: Properties of each product.

Id	Name	SBO
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k1} \cdot [\mathrm{s172}] \tag{17}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.002		☑

8.5 Reaction re5

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

Name re5

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{s46,\ s28,\ s46}} \mathrm{s32} \tag{18}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 23: Properties of each modifier.

Id	Name	SBO
s46	PXR_GENE	
s28	S_RNA	
s46	PXR_GENE	

Id	Name	SBO

Product

Table 24: Properties of each product.

Id	Name	SBO
s32	PXR_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}\,(\text{default}) \cdot \text{mRNA}\,([\text{s28}], [\text{s46}], \text{Ka}) \tag{19}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{20}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{21}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ka	Ka		$5.52 \cdot 10^{-5}$		☑

8.6 Reaction re6

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

Name re6

Reaction equation

$$\text{s32} \xrightarrow{\text{s32}} \text{s30} \tag{22}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
s32	PXR_RNA	

Modifier

Table 27: Properties of each modifier.

Id	Name	SBO
s32	PXR_RNA	

Product

Table 28: Properties of each product.

Id	Name	SBO
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k1} \cdot [\mathrm{s32}] \tag{23}$$

Table 29: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.006		☑

8.7 Reaction re7

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

Name re7

Reaction equation

$$\mathrm{s36} \xrightarrow{\mathrm{s32,\ s36,\ s32}} \mathrm{s42} \tag{24}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
s36	S_PROT	

Id	Name	SBO

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
s32	PXR_RNA	
s36	S_PROT	
s32	PXR_RNA	

Product

Table 32: Properties of each product.

Id	Name	SBO
s42	PXR_PROT	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{ptotein}\,(\mathrm{Ka}, [\mathrm{s36}], [\mathrm{s32}]) \tag{25}$$

$$\mathrm{ptotein}\,(\mathrm{Ka}, \mathrm{S\_PROT}, \mathrm{Activator}) = \mathrm{Ka} \cdot \mathrm{S\_PROT} \cdot \mathrm{Activator} \tag{26}$$

$$\mathrm{ptotein}\,(\mathrm{Ka}, \mathrm{S\_PROT}, \mathrm{Activator}) = \mathrm{Ka} \cdot \mathrm{S\_PROT} \cdot \mathrm{Activator} \tag{27}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ka	Ka		10.0		☑

8.8 Reaction re8

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

Name re8

Reaction equation

$$\text{s42} \xrightarrow{\text{s42}} \text{s30} \tag{28}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
s42	PXR_PROT	

Modifier

Table 35: Properties of each modifier.

Id	Name	SBO
s42	PXR_PROT	

Product

Table 36: Properties of each product.

Id	Name	SBO
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}\,(\text{default}) \cdot \text{k1} \cdot [\text{s42}] \tag{29}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.003		☑

8.9 Reaction re9

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

Name re9

Reaction equation

$$\text{s28} \xrightarrow{\text{s40, s28, s40}} \text{s33} \tag{30}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 39: Properties of each modifier.

Id	Name	SBO
s40	GR_GENE	
s28	S_RNA	
s40	GR_GENE	

Product

Table 40: Properties of each product.

Id	Name	SBO
s33	GR_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}\left(\text{default}\right) \cdot \text{mRNA}\left([\text{s28}], [\text{s40}], \text{Ka}\right) \tag{31}$$

$$\text{mRNA}\left(\text{S\_RNA}, \text{Activator}, \text{Ka}\right) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{32}$$

$$\text{mRNA}\left(\text{S\_RNA}, \text{Activator}, \text{Ka}\right) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{33}$$

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ka	Ka		$3.2 \cdot 10^{-6}$		☑

8.10 Reaction re10

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

Name re10

Reaction equation

$$\text{s33} \xrightarrow{\text{s33}} \text{s30} \tag{34}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
s33	GR_RNA	

Modifier

Table 43: Properties of each modifier.

Id	Name	SBO
s33	GR_RNA	

Product

Table 44: Properties of each product.

Id	Name	SBO
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}\,(\text{default}) \cdot \text{k1} \cdot [\text{s33}] \tag{35}$$

Table 45: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.003		☑

8.11 Reaction re11

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

Name re11

Reaction equation

$$\text{s36} \xrightarrow{\text{s33, s36, s33}} \text{s39} \tag{36}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
s36	S_PROT	

Modifiers

Table 47: Properties of each modifier.

Id	Name	SBO
s33	GR_RNA	
s36	S_PROT	
s33	GR_RNA	

Product

Table 48: Properties of each product.

Id	Name	SBO
s39	GR_PROT	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{ptotein}\,(\mathrm{Ka}, [\mathrm{s36}], [\mathrm{s33}]) \tag{37}$$

$$\mathrm{ptotein}\,(\mathrm{Ka}, \mathrm{S\_PROT}, \mathrm{Activator}) = \mathrm{Ka} \cdot \mathrm{S\_PROT} \cdot \mathrm{Activator} \tag{38}$$

$$\mathrm{ptotein}\,(\mathrm{Ka}, \mathrm{S\_PROT}, \mathrm{Activator}) = \mathrm{Ka} \cdot \mathrm{S\_PROT} \cdot \mathrm{Activator} \tag{39}$$

Table 49: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ka	Ka		19.98		☑

8.12 Reaction re12

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

Name re12

Reaction equation

$$\mathrm{s39} \xrightarrow{\mathrm{s39}} \mathrm{s30} \tag{40}$$

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
s39	GR_PROT	

Modifier

Table 51: Properties of each modifier.

Id	Name	SBO
s39	GR_PROT	

Product

Table 52: Properties of each product.

Id	Name	SBO
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k1} \cdot [\mathrm{s39}] \tag{41}$$

Table 53: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.001		☑

8.13 Reaction re13

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

Name re13

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{s178,\ s28,\ s178}} \mathrm{s185} \tag{42}$$

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 55: Properties of each modifier.

Id	Name	SBO
s178	TAT_GENE	
s28	S_RNA	
s178	TAT_GENE	

Id	Name	SBO

Product

Table 56: Properties of each product.

Id	Name	SBO
s185	TAT_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{mRNA}\,([\mathrm{s28}], [\mathrm{s178}], \mathrm{Ka}) \tag{43}$$

$$\mathrm{mRNA}\,(\mathrm{S\_RNA}, \mathrm{Activator}, \mathrm{Ka}) = \mathrm{Ka} \cdot \mathrm{S\_RNA} \cdot \mathrm{Activator} \tag{44}$$

$$\mathrm{mRNA}\,(\mathrm{S\_RNA}, \mathrm{Activator}, \mathrm{Ka}) = \mathrm{Ka} \cdot \mathrm{S\_RNA} \cdot \mathrm{Activator} \tag{45}$$

Table 57: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ka	Ka		$8.55 \cdot 10^{-4}$		☑

8.14 Reaction re14

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

Name re14

Reaction equation

$$\mathrm{s185} \xrightarrow{\mathrm{s185}} \mathrm{s30} \tag{46}$$

Reactant

Table 58: Properties of each reactant.

Id	Name	SBO
s185	TAT_RNA	

Modifier

Table 59: Properties of each modifier.

Id	Name	SBO
s185	TAT_RNA	

Product

Table 60: Properties of each product.

Id	Name	SBO
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k1} \cdot [\mathrm{s185}] \tag{47}$$

Table 61: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.064		☑

8.15 Reaction re15

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

Name re15

Reaction equation

$$\mathrm{s114} + \mathrm{s39} \overset{\mathrm{s114,\ s39,\ s87}}{\rightleftharpoons} \mathrm{s87} \tag{48}$$

Reactants

Table 62: Properties of each reactant.

Id	Name	SBO
s114	Cort	

Id	Name	SBO
s39	GR_PROT	

Modifiers

Table 63: Properties of each modifier.

Id	Name	SBO
s114	Cort	
s39	GR_PROT	
s87	GRprot_Cort	

Product

Table 64: Properties of each product.

Id	Name	SBO
s87	GRprot_Cort	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{k1} \cdot [\mathrm{s114}] \cdot [\mathrm{s39}] - \mathrm{k2} \cdot [\mathrm{s87}]) \tag{49}$$

Table 65: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		60.0		☑
k2	k2		600.0		☑

8.16 Reaction re16

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

Name re16

Reaction equation

$$\mathrm{s87} \xrightarrow{\mathrm{s87}} \mathrm{s114} + \mathrm{s30} \tag{50}$$

Reactant

Table 66: Properties of each reactant.

Id	Name	SBO
s87	GRprot_Cort	

Modifier

Table 67: Properties of each modifier.

Id	Name	SBO
s87	GRprot_Cort	

Products

Table 68: Properties of each product.

Id	Name	SBO
s114	Cort	
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k1} \cdot [\mathrm{s87}] \tag{51}$$

Table 69: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.001		☑

8.17 Reaction re17

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

Name re17

Reaction equation

$$\mathrm{s42} + \mathrm{s114} \xrightleftharpoons{\mathrm{s42,\ s114,\ s119}} \mathrm{s119} \tag{52}$$

Reactants

Table 70: Properties of each reactant.

Id	Name	SBO
s42	PXR_PROT	
s114	Cort	

Modifiers

Table 71: Properties of each modifier.

Id	Name	SBO
s42	PXR_PROT	
s114	Cort	
s119	PXRprot_Cort	

Product

Table 72: Properties of each product.

Id	Name	SBO
s119	PXRprot_Cort	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{k1} \cdot [\mathrm{s42}] \cdot [\mathrm{s114}] - \mathrm{k2} \cdot [\mathrm{s119}]) \tag{53}$$

Table 73: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		60.0		☑
k2	k2		600000.0		☑

8.18 Reaction re18

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

Name re18

Reaction equation

$$\mathrm{s119} \xrightarrow{\mathrm{s119}} \mathrm{s114} + \mathrm{s30} \tag{54}$$

Reactant

Table 74: Properties of each reactant.

Id	Name	SBO
s119	PXRprot_Cort	

Modifier

Table 75: Properties of each modifier.

Id	Name	SBO
s119	PXRprot_Cort	

Products

Table 76: Properties of each product.

Id	Name	SBO
s114	Cort	
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k1} \cdot [\mathrm{s119}] \tag{55}$$

Table 77: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.002		☑

8.19 Reaction re19

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

Name re19

Reaction equation

$$\text{s114} \xrightarrow{\text{s172, Ligand2, DEX, s172, s114, Ligand2, DEX}} \text{s10} \tag{56}$$

Reactant

Table 78: Properties of each reactant.

Id	Name	SBO
s114	Cort	

Modifiers

Table 79: Properties of each modifier.

Id	Name	SBO
s172	CYP_PROT	
Ligand2	Ligand2	
DEX	DEX	
s172	CYP_PROT	
s114	Cort	
Ligand2	Ligand2	
DEX	DEX	

Product

Table 80: Properties of each product.

Id	Name	SBO
s10	Cort_degr	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{LigandDegrOld}\,([\mathrm{s172}], \mathrm{Vm}, [\mathrm{s114}], \mathrm{Kms1}, [\mathrm{Ligand2}], \mathrm{Kms2}, [\mathrm{DEX}], \mathrm{Kms3}) \tag{57}$$

$$\mathrm{LigandDegrOld}\,(\mathrm{Act}, \mathrm{Vm}, \mathrm{S1}, \mathrm{Kms1}, \mathrm{S2}, \mathrm{Kms2}, \mathrm{S3}, \mathrm{Kms3}) = \mathrm{Act} \cdot \frac{\frac{\mathrm{Vm} \cdot \mathrm{S1}}{\mathrm{Kms1}}}{1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}}} \tag{58}$$

$$\mathrm{LigandDegrOld}\,(\mathrm{Act}, \mathrm{Vm}, \mathrm{S1}, \mathrm{Kms1}, \mathrm{S2}, \mathrm{Kms2}, \mathrm{S3}, \mathrm{Kms3}) = \mathrm{Act} \cdot \frac{\frac{\mathrm{Vm} \cdot \mathrm{S1}}{\mathrm{Kms1}}}{1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}}} \tag{59}$$

Table 81: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm		0.083		☑
Kms1	Kms1		15000.000		☑
Kms2	Kms2		15000.000		☑
Kms3	Kms3		23000.000		☑

8.20 Reaction re20

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

Name re20

Reaction equation

$$\mathrm{s155} + \mathrm{s119} \xrightleftharpoons{\mathrm{s155,\ s119,\ s165}} \mathrm{s165} \tag{60}$$

Reactants

Table 82: Properties of each reactant.

Id	Name	SBO
s155	CYP_GENE	
s119	PXRprot_Cort	

Modifiers

Table 83: Properties of each modifier.

Id	Name	SBO
s155	CYP_GENE	
s119	PXRprot_Cort	
s165	CYPgene_PXRprot_Cort	

Product

Table 84: Properties of each product.

Id	Name	SBO
s165	CYPgene_PXRprot_Cort	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{GeneProteinBinding\_diff\_limited} \cdot [\mathrm{s155}] \cdot [\mathrm{s119}] - \mathrm{cypGene\_PXRprotein} \cdot [\mathrm{s165}]) \tag{61}$$

8.21 Reaction re21

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

Name re21

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{s165,\ s28,\ s165}} \mathrm{s173} \tag{62}$$

Reactant

Table 85: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 86: Properties of each modifier.

Id	Name	SBO
s165	CYPgene_PXRprot_Cort	
s28	S_RNA	
s165	CYPgene_PXRprot_Cort	

Product

Table 87: Properties of each product.

Id	Name	SBO
s173	CYP_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{vol}\,(\text{default}) \cdot \text{mRNA}\,([\text{s28}], [\text{s165}], \text{cypMrna\_synt}) \tag{63}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{64}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{65}$$

8.22 Reaction re22

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

Name re22

Reaction equation

$$\text{s46} + \text{s87} \xrightleftharpoons{\text{s46, s87, s109}} \text{s109} \tag{66}$$

Reactants

Table 88: Properties of each reactant.

Id	Name	SBO
s46	PXR_GENE	
s87	GRprot_Cort	

Modifiers

Table 89: Properties of each modifier.

Id	Name	SBO
s46	PXR_GENE	
s87	GRprot_Cort	
s109	PXRgene_GRprot_Cort	

Product

Table 90: Properties of each product.

Id	Name	SBO
s109	PXRgene_GRprot_Cort	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{GeneProteinBinding\_diff\_limited} \cdot [\mathrm{s46}] \cdot [\mathrm{s87}] - \mathrm{PXRGene\_GRprotein} \cdot [\mathrm{s109}]) \tag{67}$$

8.23 Reaction re23

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

Name re23

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{s109,\ s28,\ s109}} \mathrm{s32} \tag{68}$$

Reactant

Table 91: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 92: Properties of each modifier.

Id	Name	SBO
s109	PXRgene_GRprot_Cort	
s28	S_RNA	
s109	PXRgene_GRprot_Cort	

Product

Table 93: Properties of each product.

Id	Name	SBO
s32	PXR_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{mRNA}\,([\mathrm{s28}], [\mathrm{s109}], \mathrm{pxrMrna\_synt}) \tag{69}$$

$$\mathrm{mRNA}\,(\mathrm{S\_RNA}, \mathrm{Activator}, \mathrm{Ka}) = \mathrm{Ka} \cdot \mathrm{S\_RNA} \cdot \mathrm{Activator} \tag{70}$$

$$\mathrm{mRNA}\,(\mathrm{S\_RNA}, \mathrm{Activator}, \mathrm{Ka}) = \mathrm{Ka} \cdot \mathrm{S\_RNA} \cdot \mathrm{Activator} \tag{71}$$

8.24 Reaction re24

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

Name re24

Reaction equation

$$\mathrm{s40} + \mathrm{s87} \overset{\mathrm{s40,\ s87,\ s84}}{\rightleftharpoons} \mathrm{s84} \tag{72}$$

Reactants

Table 94: Properties of each reactant.

Id	Name	SBO
s40	GR_GENE	
s87	GRprot_Cort	

Modifiers

Table 95: Properties of each modifier.

Id	Name	SBO
s40	GR_GENE	
s87	GRprot_Cort	
s84	GRgene_GRprot_Cort	

Product

Table 96: Properties of each product.

Id	Name	SBO
s84	GRgene_GRprot_Cort	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{GeneProteinBinding\_diff\_limited} \cdot [\mathrm{s40}] \cdot [\mathrm{s87}] - \mathrm{GRGene\_GRprotein} \cdot [\mathrm{s84}]) \tag{73}$$

8.25 Reaction re25

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

Name re25

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{s84,\ s28,\ s84}} \mathrm{s33} \tag{74}$$

Reactant

Table 97: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 98: Properties of each modifier.

Id	Name	SBO
s84	GRgene_GRprot_Cort	
s28	S_RNA	
s84	GRgene_GRprot_Cort	

Product

Table 99: Properties of each product.

Id	Name	SBO
s33	GR_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \text{vol}\,(\text{default}) \cdot \text{mRNA}\,([\text{s28}], [\text{s84}], \text{grMrna\_synt}) \tag{75}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{76}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{77}$$

8.26 Reaction re26

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

Name re26

Reaction equation

$$\text{s178} + \text{s87} \xrightleftharpoons{\text{s178, s87, s183}} \text{s183} \tag{78}$$

Reactants

Table 100: Properties of each reactant.

Id	Name	SBO
s178	TAT_GENE	
s87	GRprot_Cort	

Modifiers

Table 101: Properties of each modifier.

Id	Name	SBO
s178	TAT_GENE	
s87	GRprot_Cort	
s183	TATgene_GRprot_Cort	

Product

Table 102: Properties of each product.

Id	Name	SBO
s183	TATgene_GRprot_Cort	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{GeneProteinBinding\_diff\_limited} \cdot [\mathrm{s178}] \cdot [\mathrm{s87}] - \mathrm{TATGene\_GRprotein} \cdot [\mathrm{s183}]) \tag{79}$$

8.27 Reaction re27

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

Name re27

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{s183,\ s28,\ s183}} \mathrm{s185} \tag{80}$$

Reactant

Table 103: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 104: Properties of each modifier.

Id	Name	SBO
s183	TATgene_GRprot_Cort	
s28	S_RNA	
s183	TATgene_GRprot_Cort	

Product

Table 105: Properties of each product.

Id	Name	SBO
s185	TAT_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \text{vol}\,(\text{default}) \cdot \text{mRNA}\,([\text{s28}], [\text{s183}], \text{tatMrna\_synt}) \tag{81}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{82}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{83}$$

8.28 Reaction re42

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

Name re42

Reaction equation

$$\text{Cortisone} \overset{\text{Cortisone, s114}}{\rightleftharpoons} \text{s114} \tag{84}$$

Reactant

Table 106: Properties of each reactant.

Id	Name	SBO
Cortisone	Cortisone	

Modifiers

Table 107: Properties of each modifier.

Id	Name	SBO
Cortisone	Cortisone	
s114	Cort	

Product

Table 108: Properties of each product.

Id	Name	SBO
s114	Cort	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{k1} \cdot [\mathrm{Cortisone}] - \mathrm{k2} \cdot [\mathrm{s114}]) \tag{85}$$

Table 109: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.016		☑
k2	k2		0.016		☑

8.29 Reaction re44

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

Name re44

Reaction equation

$$\mathrm{TAT\_PROT} \xrightarrow{\mathrm{TAT\_PROT}} \mathrm{s30} \tag{86}$$

Reactant

Table 110: Properties of each reactant.

Id	Name	SBO
TAT_PROT	TAT_PROT	

Modifier

Table 111: Properties of each modifier.

Id	Name	SBO
TAT_PROT	TAT_PROT	

Product

Table 112: Properties of each product.

Id	Name	SBO
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k1} \cdot [\mathrm{TAT\_PROT}] \tag{87}$$

Table 113: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.012		☑

8.30 Reaction re43

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

Name re43

Reaction equation

$$\text{s36} \xrightarrow{\text{s185, s36, s185}} \text{TAT\_PROT} \tag{88}$$

Reactant

Table 114: Properties of each reactant.

Id	Name	SBO
s36	S_PROT	

Modifiers

Table 115: Properties of each modifier.

Id	Name	SBO
s185	TAT_RNA	
s36	S_PROT	
s185	TAT_RNA	

Product

Table 116: Properties of each product.

Id	Name	SBO
TAT_PROT	TAT_PROT	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \text{vol}\left(\text{default}\right) \cdot \text{ptotein}\left(\text{Ka}, [\text{s36}], [\text{s185}]\right) \tag{89}$$

$$\text{ptotein}\left(\text{Ka}, \text{S\_PROT}, \text{Activator}\right) = \text{Ka} \cdot \text{S\_PROT} \cdot \text{Activator} \tag{90}$$

$$\text{ptotein}\left(\text{Ka}, \text{S\_PROT}, \text{Activator}\right) = \text{Ka} \cdot \text{S\_PROT} \cdot \text{Activator} \tag{91}$$

Table 117: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ka	Ka		0.5		☑

8.31 Reaction cortisolTransport

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

Name cortisolTransport

Reaction equation

$$\mathrm{s2} \overset{\mathrm{s2,\ s114}}{\rightleftharpoons} \mathrm{s114} \tag{92}$$

Reactant

Table 118: Properties of each reactant.

Id	Name	SBO
s2	CortOUT	

Modifiers

Table 119: Properties of each modifier.

Id	Name	SBO
s2	CortOUT	
s114	Cort	

Product

Table 120: Properties of each product.

Id	Name	SBO
s114	Cort	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \mathrm{k1} \cdot [\mathrm{s2}] - \mathrm{k2} \cdot [\mathrm{s114}] \tag{93}$$

Table 121: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		1000.0		☑
k2	k2		1000.0		☑

8.32 Reaction L2_PXR_binding

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

Name L2_PXR_binding

Reaction equation

$$\mathrm{s42} + \mathrm{Ligand2} \underset{}{\overset{\mathrm{s42,\ Ligand2,\ PXRprot\_Ligand2}}{\rightleftharpoons}} \mathrm{PXRprot\_Ligand2} \tag{94}$$

Reactants

Table 122: Properties of each reactant.

Id	Name	SBO
s42	PXR_PROT	
Ligand2	Ligand2	

Modifiers

Table 123: Properties of each modifier.

Id	Name	SBO
s42	PXR_PROT	
Ligand2	Ligand2	
PXRprot_Ligand2	PXRprot_Ligand2	

Product

Table 124: Properties of each product.

Id	Name	SBO
PXRprot_Ligand2	PXRprot_Ligand2	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{k1} \cdot [\mathrm{s42}] \cdot [\mathrm{Ligand2}] - \mathrm{k2} \cdot [\mathrm{PXRprot\_Ligand2}]) \tag{95}$$

Table 125: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		60.0		☑
k2	k2		600000.0		☑

8.33 Reaction L2_PXR_deg

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

Name L2_PXR_deg

Reaction equation

$$\mathrm{PXRprot\_Ligand2} \xrightarrow{\mathrm{PXRprot\_Ligand2}} \mathrm{Ligand2} + \mathrm{s30} \tag{96}$$

Reactant

Table 126: Properties of each reactant.

Id	Name	SBO
PXRprot_Ligand2	PXRprot_Ligand2	

Modifier

Table 127: Properties of each modifier.

Id	Name	SBO
PXRprot_Ligand2	PXRprot_Ligand2	

Products

Table 128: Properties of each product.

Id	Name	SBO
Ligand2	Ligand2	
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k1} \cdot [\mathrm{PXRprot\_Ligand2}] \tag{97}$$

Table 129: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.002		☑

8.34 Reaction CYPmRNA_synt_PXR_L2

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

Name CYPmRNA_synt_PXR_L2

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{CYPgene\_PXRprot\_Ligand2,\ s28,\ CYPgene\_PXRprot\_Ligand2}} \mathrm{s173} \tag{98}$$

Reactant

Table 130: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 131: Properties of each modifier.

Id	Name	SBO
CYPgene_PXRprot_Ligand2	CYPgene_PXRprot_Ligand2	
s28	S_RNA	
CYPgene_PXRprot_Ligand2	CYPgene_PXRprot_Ligand2	

Product

Table 132: Properties of each product.

Id	Name	SBO
s173	CYP_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \text{vol}\,(\text{default}) \cdot \text{mRNA}\,([\text{s28}], [\text{CYPgene\_PXRprot\_Ligand2}], \text{cypMrna\_synt}) \quad (99)$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \quad (100)$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \quad (101)$$

8.35 Reaction CYPmRNA_PXR_L2_binding

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

Name CYPmRNA_PXR_L2_binding

Reaction equation

$$\text{s155} + \text{PXRprot\_Ligand2} \xrightleftharpoons{\text{s155, PXRprot\_Ligand2, CYPgene\_PXRprot\_Ligand2}} \text{CYPgene\_PXRprot\_Ligand2} \quad (102)$$

Reactants

Table 133: Properties of each reactant.

Id	Name	SBO
s155	CYP_GENE	
PXRprot_Ligand2	PXRprot_Ligand2	

Modifiers

Table 134: Properties of each modifier.

Id	Name	SBO
s155	CYP_GENE	
PXRprot_Ligand2	PXRprot_Ligand2	
CYPgene_PXRprot_Ligand2	CYPgene_PXRprot_Ligand2	

Product

Table 135: Properties of each product.

Id	Name	SBO
CYPgene_PXRprot_Ligand2	CYPgene_PXRprot_Ligand2	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{GeneProteinBinding\_diff\_limited} \cdot [\mathrm{s155}] \cdot [\mathrm{PXRprot\_Ligand2}] - \mathrm{cypGene\_PXRprotein} \cdot [\mathrm{CYPgene\_PXRprot\_Ligand2}]) \quad (103)$$

8.36 Reaction re28

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

Name re28

Reaction equation

$$\mathrm{s39} + \mathrm{DEX} \overset{\text{s39, DEX, GRprot\_DEX}}{\rightleftharpoons} \mathrm{GRprot\_DEX} \quad (104)$$

Reactants

Table 136: Properties of each reactant.

Id	Name	SBO
s39	GR_PROT	
DEX	DEX	

Modifiers

Table 137: Properties of each modifier.

Id	Name	SBO
s39	GR_PROT	
DEX	DEX	
GRprot_DEX	GRprot_DEX	

Product

Table 138: Properties of each product.

Id	Name	SBO
GRprot_DEX	GRprot_DEX	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{k1} \cdot [\mathrm{s39}] \cdot [\mathrm{DEX}] - \mathrm{k2} \cdot [\mathrm{GRprot\_DEX}]) \tag{105}$$

Table 139: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		60.0		☑
k2	k2		60.0		☑

8.37 Reaction re29

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

Name re29

Reaction equation

$$\mathrm{GRprot\_DEX} \xrightarrow{\mathrm{GRprot\_DEX}} \mathrm{s30} + \mathrm{DEX} \tag{106}$$

Reactant

Table 140: Properties of each reactant.

Id	Name	SBO
GRprot_DEX	GRprot_DEX	

Modifier

Table 141: Properties of each modifier.

Id	Name	SBO
GRprot_DEX	GRprot_DEX	

Products

Table 142: Properties of each product.

Id	Name	SBO
s30	P	
DEX	DEX	

Kinetic Law

Derived unit contains undeclared units

$$v_{37} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k1} \cdot [\mathrm{GRprot\_DEX}] \tag{107}$$

Table 143: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.001		☑

8.38 Reaction re30

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

Name re30

Reaction equation

$$\mathrm{s42} + \mathrm{DEX} \xrightleftharpoons{\text{s42, DEX, PXRprot\_DEX}} \mathrm{PXRprot\_DEX} \tag{108}$$

Reactants

Table 144: Properties of each reactant.

Id	Name	SBO
s42	PXR_PROT	
DEX	DEX	

Modifiers

Table 145: Properties of each modifier.

Id	Name	SBO
s42	PXR_PROT	
DEX	DEX	
PXRprot_DEX	PXRprot_DEX	

Product

Table 146: Properties of each product.

Id	Name	SBO
PXRprot_DEX	PXRprot_DEX	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{k1} \cdot [\mathrm{s42}] \cdot [\mathrm{DEX}] - \mathrm{k2} \cdot [\mathrm{PXRprot\_DEX}]) \tag{109}$$

Table 147: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		60.0		☑
k2	k2		60000.0		☑

8.39 Reaction re31

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

Name re31

Reaction equation

$$\text{PXRprot\_DEX} \xrightarrow{\text{PXRprot\_DEX}} \text{DEX} + \text{s30} \tag{110}$$

Reactant

Table 148: Properties of each reactant.

Id	Name	SBO
PXRprot_DEX	PXRprot_DEX	

Modifier

Table 149: Properties of each modifier.

Id	Name	SBO
PXRprot_DEX	PXRprot_DEX	

Products

Table 150: Properties of each product.

Id	Name	SBO
DEX	DEX	
s30	P	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = \text{vol}\,(\text{default}) \cdot \text{k1} \cdot [\text{PXRprot\_DEX}] \tag{111}$$

Table 151: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.002		☑

8.40 Reaction re32

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

Name re32

Reaction equation

$$\text{DEX} \xrightarrow{\text{s172, Ligand2, s114, s172, DEX, Ligand2, s114}} \text{DEX\_degr} \tag{112}$$

Reactant

Table 152: Properties of each reactant.

Id	Name	SBO
DEX	DEX	

Modifiers

Table 153: Properties of each modifier.

Id	Name	SBO
s172	CYP_PROT	
Ligand2	Ligand2	
s114	Cort	
s172	CYP_PROT	
DEX	DEX	
Ligand2	Ligand2	
s114	Cort	

Product

Table 154: Properties of each product.

Id	Name	SBO
DEX_degr	DEX_degr	

Kinetic Law

Derived unit contains undeclared units

$$v_{40} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{LigandDegrOld}\,([\mathrm{s172}], \mathrm{Vm}, [\mathrm{DEX}], \mathrm{Kms1}, [\mathrm{Ligand2}], \mathrm{Kms2}, [\mathrm{s114}], \mathrm{Kms3}) \tag{113}$$

$$\mathrm{LigandDegrOld}\,(\mathrm{Act}, \mathrm{Vm}, \mathrm{S1}, \mathrm{Kms1}, \mathrm{S2}, \mathrm{Kms2}, \mathrm{S3}, \mathrm{Kms3}) = \mathrm{Act} \cdot \frac{\frac{\mathrm{Vm} \cdot \mathrm{S1}}{\mathrm{Kms1}}}{1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}}} \tag{114}$$

$$\mathrm{LigandDegrOld}\,(\mathrm{Act}, \mathrm{Vm}, \mathrm{S1}, \mathrm{Kms1}, \mathrm{S2}, \mathrm{Kms2}, \mathrm{S3}, \mathrm{Kms3}) = \mathrm{Act} \cdot \frac{\frac{\mathrm{Vm} \cdot \mathrm{S1}}{\mathrm{Kms1}}}{1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}}} \tag{115}$$

Table 155: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Vm`	Vm		0.004		☑
`Kms1`	Kms1		23000.000		☑
`Kms2`	Kms2		15000.000		☑
`Kms3`	Kms3		15000.000		☑

8.41 Reaction `re33`

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

Name re33

Reaction equation

$$\mathrm{s155} + \mathrm{PXRprot\_DEX} \xrightleftharpoons{\text{s155, PXRprot\_DEX, CYPgene\_PXRprot\_DEX}} \mathrm{CYPgene\_PXRprot\_DEX} \tag{116}$$

Reactants

Table 156: Properties of each reactant.

Id	Name	SBO
`s155`	CYP_GENE	
`PXRprot_DEX`	PXRprot_DEX	

Modifiers

Table 157: Properties of each modifier.

Id	Name	SBO
s155	CYP_GENE	
PXRprot_DEX	PXRprot_DEX	
CYPgene_PXRprot_DEX	CYPgene_PXRprot_DEX	

Product

Table 158: Properties of each product.

Id	Name	SBO
CYPgene_PXRprot_DEX	CYPgene_PXRprot_DEX	

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{GeneProteinBinding\_diff\_limited} \cdot [\mathrm{s155}] \cdot [\mathrm{PXRprot\_DEX}] - \mathrm{cypGene\_PXRprotein} \cdot [\mathrm{CYPgene\_PXRprot\_DEX}]) \quad (117)$$

8.42 Reaction re34

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

Name re34

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{CYPgene\_PXRprot\_DEX,\ s28,\ CYPgene\_PXRprot\_DEX}} \mathrm{s173} \quad (118)$$

Reactant

Table 159: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 160: Properties of each modifier.

Id	Name	SBO
CYPgene_PXRprot_DEX	CYPgene_PXRprot_DEX	
s28	S_RNA	
CYPgene_PXRprot_DEX	CYPgene_PXRprot_DEX	

Product

Table 161: Properties of each product.

Id	Name	SBO
s173	CYP_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = \text{vol}\,(\text{default}) \cdot \text{mRNA}\,([\text{s28}], [\text{CYPgene\_PXRprot\_DEX}], \text{cypMrna\_synt}) \quad (119)$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \quad (120)$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \quad (121)$$

8.43 Reaction re35

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

Name re35

Reaction equation

$$\text{GRprot\_DEX} + \text{s46} \xrightleftharpoons{\text{GRprot\_DEX, s46, PXRgene\_GRprot\_DEX}} \text{PXRgene\_GRprot\_DEX} \quad (122)$$

Reactants

Table 162: Properties of each reactant.

Id	Name	SBO
GRprot_DEX	GRprot_DEX	
s46	PXR_GENE	

Modifiers

Table 163: Properties of each modifier.

Id	Name	SBO
GRprot_DEX	GRprot_DEX	
s46	PXR_GENE	
PXRgene_GRprot_DEX	PXRgene_GRprot_DEX	

Product

Table 164: Properties of each product.

Id	Name	SBO
PXRgene_GRprot_DEX	PXRgene_GRprot_DEX	

Kinetic Law

Derived unit contains undeclared units

$$v_{43} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{GeneProteinBinding\_diff\_limited} \cdot [\mathrm{GRprot\_DEX}] \cdot [\mathrm{s46}] - \mathrm{PXRGene\_GRprotein} \cdot [\mathrm{PXRgene\_GRprot\_DEX}]) \quad (123)$$

8.44 Reaction re36

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

Name re36

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{PXRgene\_GRprot\_DEX,\ s28,\ PXRgene\_GRprot\_DEX}} \mathrm{s32} \quad (124)$$

Reactant

Table 165: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 166: Properties of each modifier.

Id	Name	SBO
PXRgene_GRprot_DEX	PXRgene_GRprot_DEX	
s28	S_RNA	
PXRgene_GRprot_DEX	PXRgene_GRprot_DEX	

Product

Table 167: Properties of each product.

Id	Name	SBO
s32	PXR_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{44} = \text{vol}\,(\text{default}) \cdot \text{mRNA}\,([\text{s28}], [\text{PXRgene\_GRprot\_DEX}], \text{pxrMrna\_synt}) \quad (125)$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \quad (126)$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \quad (127)$$

8.45 Reaction re37

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

Name re37

Reaction equation

$$\text{GRprot\_DEX} + \text{s40} \xrightleftharpoons{\text{GRprot\_DEX, s40, GRgene\_GRprot\_DEX}} \text{GRgene\_GRprot\_DEX} \quad (128)$$

Reactants

Table 168: Properties of each reactant.

Id	Name	SBO
GRprot_DEX	GRprot_DEX	
s40	GR_GENE	

Modifiers

Table 169: Properties of each modifier.

Id	Name	SBO
GRprot_DEX	GRprot_DEX	
s40	GR_GENE	
GRgene_GRprot_DEX	GRgene_GRprot_DEX	

Product

Table 170: Properties of each product.

Id	Name	SBO
GRgene_GRprot_DEX	GRgene_GRprot_DEX	

Kinetic Law

Derived unit contains undeclared units

$$v_{45} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{GeneProteinBinding\_diff\_limited} \cdot [\mathrm{GRprot\_DEX}] \cdot [\mathrm{s40}] - \mathrm{GRGene\_GRprotein} \cdot [\mathrm{GRgene\_GRprot\_DEX}]) \quad (129)$$

8.46 Reaction re38

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

Name re38

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{GRgene\_GRprot\_DEX,\ s28,\ GRgene\_GRprot\_DEX}} \mathrm{s33} \quad (130)$$

Reactant

Table 171: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 172: Properties of each modifier.

Id	Name	SBO
GRgene_GRprot_DEX	GRgene_GRprot_DEX	
s28	S_RNA	
GRgene_GRprot_DEX	GRgene_GRprot_DEX	

Product

Table 173: Properties of each product.

Id	Name	SBO
s33	GR_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{46} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{mRNA}\,([\mathrm{s28}], [\mathrm{GRgene\_GRprot\_DEX}], \mathrm{grMrna\_synt}) \tag{131}$$

$$\mathrm{mRNA}\,(\mathrm{S\_RNA}, \mathrm{Activator}, \mathrm{Ka}) = \mathrm{Ka} \cdot \mathrm{S\_RNA} \cdot \mathrm{Activator} \tag{132}$$

$$\mathrm{mRNA}\,(\mathrm{S\_RNA}, \mathrm{Activator}, \mathrm{Ka}) = \mathrm{Ka} \cdot \mathrm{S\_RNA} \cdot \mathrm{Activator} \tag{133}$$

8.47 Reaction re39

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

Name re39

Reaction equation

$$\mathrm{GRprot\_DEX} + \mathrm{s178} \xrightleftharpoons{\mathrm{GRprot\_DEX},\ \mathrm{s178},\ \mathrm{TATgene\_GRprot\_DEX}} \mathrm{TATgene\_GRprot\_DEX} \tag{134}$$

Reactants

Table 174: Properties of each reactant.

Id	Name	SBO
GRprot_DEX	GRprot_DEX	
s178	TAT_GENE	

Modifiers

Table 175: Properties of each modifier.

Id	Name	SBO
GRprot_DEX	GRprot_DEX	
s178	TAT_GENE	
TATgene_GRprot_DEX	TATgene_GRprot_DEX	

Product

Table 176: Properties of each product.

Id	Name	SBO
TATgene_GRprot_DEX	TATgene_GRprot_DEX	

Kinetic Law

Derived unit contains undeclared units

$$v_{47} = \mathrm{vol}\,(\mathrm{default}) \cdot (\mathrm{GeneProteinBinding\_diff\_limited} \cdot [\mathrm{GRprot\_DEX}] \cdot [\mathrm{s178}] - \mathrm{TATGene\_GRprotein} \cdot [\mathrm{TATgene\_GRprot\_DEX}]) \quad (135)$$

8.48 Reaction re40

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

Name re40

Reaction equation

$$\mathrm{s28} \xrightarrow{\mathrm{TATgene\_GRprot\_DEX,\ s28,\ TATgene\_GRprot\_DEX}} \mathrm{s185} \quad (136)$$

Reactant

Table 177: Properties of each reactant.

Id	Name	SBO
s28	S_RNA	

Modifiers

Table 178: Properties of each modifier.

Id	Name	SBO
TATgene_GRprot_DEX	TATgene_GRprot_DEX	
s28	S_RNA	
TATgene_GRprot_DEX	TATgene_GRprot_DEX	

Product

Table 179: Properties of each product.

Id	Name	SBO
s185	TAT_RNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{48} = \text{vol}\,(\text{default}) \cdot \text{mRNA}\,([\text{s28}], [\text{TATgene\_GRprot\_DEX}], \text{tatMrna\_synt}) \tag{137}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{138}$$

$$\text{mRNA}\,(\text{S\_RNA}, \text{Activator}, \text{Ka}) = \text{Ka} \cdot \text{S\_RNA} \cdot \text{Activator} \tag{139}$$

8.49 Reaction re41

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

Name re41

Reaction equation

$$\text{DEXout} \underset{\text{DEXout, DEX}}{\rightleftharpoons} \text{DEX} \tag{140}$$

Reactant

Table 180: Properties of each reactant.

Id	Name	SBO
DEXout	DEXout	

Modifiers

Table 181: Properties of each modifier.

Id	Name	SBO
DEXout	DEXout	
DEX	DEX	

Product

Table 182: Properties of each product.

Id	Name	SBO
DEX	DEX	

Kinetic Law

Derived unit contains undeclared units

$$v_{49} = \mathrm{k1} \cdot [\mathrm{DEXout}] - \mathrm{k2} \cdot [\mathrm{DEX}] \tag{141}$$

Table 183: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		100.0		☑
k2	k2		100.0		☑

8.50 Reaction Cortisol_CBG

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

Name Cortisol_CBG

Reaction equation

$$\mathrm{s2} + \mathrm{CBG} \xrightleftharpoons{\text{s2, CBG, CBG\_CortOUT}} \mathrm{CBG\_CortOUT} \tag{142}$$

Reactants

Table 184: Properties of each reactant.

Id	Name	SBO
s2	CortOUT	
CBG	CBG	

Modifiers

Table 185: Properties of each modifier.

Id	Name	SBO
s2	CortOUT	
CBG	CBG	
CBG_CortOUT	CBG_CortOUT	

Product

Table 186: Properties of each product.

Id	Name	SBO
CBG_CortOUT	CBG_CortOUT	

Kinetic Law

Derived unit contains undeclared units

$$v_{50} = \mathrm{vol}\,(\mathrm{blood}) \cdot (\mathrm{k1} \cdot [\mathrm{s2}] \cdot [\mathrm{CBG}] - \mathrm{k2} \cdot [\mathrm{CBG\_CortOUT}]) \tag{143}$$

Table 187: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		60.0		☑
k2	k2		270.0		☑

8.51 Reaction Cort_Alb

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

Name Cort_Alb

Reaction equation

$$\mathrm{Alb} + \mathrm{s2} \xrightleftharpoons{\text{Alb, s2, Alb\_CortOUT}} \mathrm{Alb\_CortOUT} \tag{144}$$

Reactants

Table 188: Properties of each reactant.

Id	Name	SBO
`Alb`	Alb	
`s2`	CortOUT	

Modifiers

Table 189: Properties of each modifier.

Id	Name	SBO
`Alb`	Alb	
`s2`	CortOUT	
`Alb_CortOUT`	Alb_CortOUT	

Product

Table 190: Properties of each product.

Id	Name	SBO
`Alb_CortOUT`	Alb_CortOUT	

Kinetic Law

Derived unit contains undeclared units

$$v_{51} = \mathrm{vol}\,(\mathrm{blood}) \cdot (\mathrm{k1} \cdot [\mathrm{Alb}] \cdot [\mathrm{s2}] - \mathrm{k2} \cdot [\mathrm{Alb\_CortOUT}]) \tag{145}$$

Table 191: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`k1`	k1		60.0		☑
`k2`	k2		900000.0		☑

8.52 Reaction cort_distribution

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

Name cort_distribution

Reaction equation

$$\text{CortAdded} \xrightarrow{\text{CortAdded}} \text{s2} \tag{146}$$

Reactant

Table 192: Properties of each reactant.

Id	Name	SBO
CortAdded	CortAdded	

Modifier

Table 193: Properties of each modifier.

Id	Name	SBO
CortAdded	CortAdded	

Product

Table 194: Properties of each product.

Id	Name	SBO
s2	CortOUT	

Kinetic Law

Derived unit contains undeclared units

$$v_{52} = \text{vol}(\text{blood}) \cdot \text{k1} \cdot [\text{CortAdded}] \tag{147}$$

Table 195: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		1000.0		☑

9 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.

9.1 Species s28

Name S_RNA

Initial concentration $1.00000029723653\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in 26 reactions (as a reactant in re1, re5, re9, re13, re21, re23, re25, re27, CYPmRNA_synt_PXR_L2, re34, re36, re38, re40 and as a modifier in re1, re5, re9, re13, re21, re23, re25, re27, CYPmRNA_synt_PXR_L2, re34, re36, re38, re40), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s28} = 0 \tag{148}$$

9.2 Species s36

Name S_PROT

Initial concentration $1.00000029723653\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in re3, re7, re11, re43 and as a modifier in re3, re7, re11, re43), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s36} = 0 \tag{149}$$

9.3 Species s46

Name PXR_GENE

Initial concentration $0.780000231844494\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in re22, re35 and as a modifier in re5, re5, re22, re35).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s46} = -\,v_{22} - v_{43} \tag{150}$$

9.4 Species s32

Name PXR_RNA

Initial concentration $0.00700000208065571\ \text{nmol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in re6 and as a product in re5, re23, re36 and as a modifier in re6, re7, re7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{s32} = v_5 + v_{23} + v_{44} - v_6 \tag{151}$$

9.5 Species s42

Name PXR_PROT

Initial concentration $99.9000296939294\ \text{nmol} \cdot \text{l}^{-1}$

This species takes part in nine reactions (as a reactant in re8, re17, L2_PXR_binding, re30 and as a product in re7 and as a modifier in re8, re17, L2_PXR_binding, re30).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{s42} = v_7 - v_8 - v_{17} - v_{32} - v_{38} \tag{152}$$

9.6 Species s30

Name P

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

This species takes part in 13 reactions (as a product in re2, re4, re6, re8, re10, re12, re14, re16, re18, re44, L2_PXR_deg, re29, re31), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{s30} = 0 \tag{153}$$

9.7 Species s40

Name GR_GENE

Initial concentration $0.500000148618265\ \text{nmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in re24, re37 and as a modifier in re9, re9, re24, re37).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{s40} = -v_{24} - v_{45} \tag{154}$$

9.8 Species s33

Name GR_RNA

Initial concentration $8.00000237789224 \cdot 10^{-4}$ nmol $\cdot$ l^{-1}

This species takes part in seven reactions (as a reactant in re10 and as a product in re9, re25, re38 and as a modifier in re10, re11, re11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s33} = v_9 + v_{25} + v_{46} - v_{10} \tag{155}$$

9.9 Species s39

Name GR_PROT

Initial concentration 47.2400140414537 nmol $\cdot$ l^{-1}

This species takes part in seven reactions (as a reactant in re12, re15, re28 and as a product in re11 and as a modifier in re12, re15, re28).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s39} = v_{11} - v_{12} - v_{15} - v_{36} \tag{156}$$

9.10 Species s114

Name Cort

Initial concentration 1.14000033884965 nmol $\cdot$ l^{-1}

This species takes part in 14 reactions (as a reactant in re15, re17, re19 and as a product in re16, re18, re42, cortisolTransport and as a modifier in re15, re17, re19, re42, cortisolTransport, re32, re32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s114} = v_{16} + v_{18} + v_{28} + v_{31} - v_{15} - v_{17} - v_{19} \tag{157}$$

9.11 Species s155

Name CYP_GENE

Initial concentration 0.829760246634984 nmol $\cdot$ l^{-1}

This species takes part in eight reactions (as a reactant in re20, CYPmRNA_PXR_L2_binding, re33 and as a modifier in re1, re1, re20, CYPmRNA_PXR_L2_binding, re33).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s155} = -v_{20} - v_{35} - v_{41} \tag{158}$$

9.12 Species s172

Name CYP_PROT

Initial concentration 104.000030912599 nmol · l^{-1}

This species takes part in seven reactions (as a reactant in re4 and as a product in re3 and as a modifier in re4, re19, re19, re32, re32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s172} = v_3 - v_4 \tag{159}$$

9.13 Species s173

Name CYP_RNA

Initial concentration 0.0750000222927398 nmol · l^{-1}

This species takes part in eight reactions (as a reactant in re2 and as a product in re1, re21, CYPmRNA_synt_PXR_L2, re34 and as a modifier in re2, re3, re3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s173} = v_1 + v_{21} + v_{34} + v_{42} - v_2 \tag{160}$$

9.14 Species s185

Name TAT_RNA

Initial concentration 0.100000029723653 nmol · l^{-1}

This species takes part in seven reactions (as a reactant in re14 and as a product in re13, re27, re40 and as a modifier in re14, re43, re43).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s185} = v_{13} + v_{27} + v_{48} - v_{14} \tag{161}$$

9.15 Species s84

Name GRgene_GRprot_Cort

Initial concentration 0.330000098088055 nmol · l^{-1}

This species takes part in four reactions (as a product in re24 and as a modifier in re24, re25, re25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s84} = v_{24} \tag{162}$$

9.16 Species s165

Name CYPgene_PXRprot_Cort

Initial concentration $2.40000071336767 \cdot 10^{-4}$ nmol $\cdot$ l^{-1}

This species takes part in four reactions (as a product in re20 and as a modifier in re20, re21, re21).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s165} = v_{20} \tag{163}$$

9.17 Species s109

Name PXRgene_GRprot_Cort

Initial concentration 0.0500000148618265 nmol $\cdot$ l^{-1}

This species takes part in four reactions (as a product in re22 and as a modifier in re22, re23, re23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s109} = v_{22} \tag{164}$$

9.18 Species s87

Name GRprot_Cort

Initial concentration 32.3600096185741 nmol $\cdot$ l^{-1}

This species takes part in ten reactions (as a reactant in re16, re22, re24, re26 and as a product in re15 and as a modifier in re15, re16, re22, re24, re26).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s87} = v_{15} - v_{16} - v_{22} - v_{24} - v_{26} \tag{165}$$

9.19 Species s119

Name PXRprot_Cort

Initial concentration 0.0100000029723653 nmol $\cdot$ l^{-1}

This species takes part in six reactions (as a reactant in re18, re20 and as a product in re17 and as a modifier in re17, re18, re20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s119} = v_{17} - v_{18} - v_{20} \tag{166}$$

9.20 Species s183

Name TATgene_GRprot_Cort

Initial concentration $0.0200000059447306\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a product in re26 and as a modifier in re26, re27, re27).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s183} = v_{26} \tag{167}$$

9.21 Species s178

Name TAT_GENE

Initial concentration $0.81000024076159\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in re26, re39 and as a modifier in re13, re13, re26, re39).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s178} = -v_{26} - v_{47} \tag{168}$$

9.22 Species s10

Name Cort_degr

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

This species takes part in one reaction (as a product in re19), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s10} = 0 \tag{169}$$

9.23 Species Cortisone

Name Cortisone

Initial concentration $24.0000071336767\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in re42 and as a modifier in re42), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cortisone} = 0 \tag{170}$$

9.24 Species TAT_PROT

Name TAT_PROT

Initial concentration $0.46202810387596\ \text{nmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in re44 and as a product in re43 and as a modifier in re44).

$$\frac{\text{d}}{\text{d}t}\text{TAT\_PROT} = v_{30} - v_{29} \tag{171}$$

9.25 Species Ligand2

Name Ligand2

Initial concentration $100.000029723653\ \text{nmol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in L2_PXR_binding and as a product in L2_PXR_deg and as a modifier in re19, re19, L2_PXR_binding, re32, re32).

$$\frac{\text{d}}{\text{d}t}\text{Ligand2} = v_{33} - v_{32} \tag{172}$$

9.26 Species PXRprot_Ligand2

Name PXRprot_Ligand2

Initial concentration $0.00100000029723653\ \text{nmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in L2_PXR_deg, CYPmRNA_PXR_L2_binding and as a product in L2_PXR_binding and as a modifier in L2_PXR_binding, L2_PXR_deg, CYPmRNA_PXR_L2_binding).

$$\frac{\text{d}}{\text{d}t}\text{PXRprot\_Ligand2} = v_{32} - v_{33} - v_{35} \tag{173}$$

9.27 Species CYPgene_PXRprot_Ligand2

Name CYPgene_PXRprot_Ligand2

Initial concentration $2.40000071336767 \cdot 10^{-5}\ \text{nmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a product in CYPmRNA_PXR_L2_binding and as a modifier in CYPmRNA_synt_PXR_L2, CYPmRNA_synt_PXR_L2, CYPmRNA_PXR_L2_binding).

$$\frac{\text{d}}{\text{d}t}\text{CYPgene\_PXRprot\_Ligand2} = v_{35} \tag{174}$$

9.28 Species DEX

Name DEX

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

This species takes part in twelve reactions (as a reactant in re28, re30, re32 and as a product in re29, re31, re41 and as a modifier in re19, re19, re28, re30, re32, re41).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DEX} = v_{37} + v_{39} + v_{49} - v_{36} - v_{38} - v_{40} \tag{175}$$

9.29 Species GRprot_DEX

Name GRprot_DEX

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

This species takes part in ten reactions (as a reactant in re29, re35, re37, re39 and as a product in re28 and as a modifier in re28, re29, re35, re37, re39).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GRprot\_DEX} = v_{36} - v_{37} - v_{43} - v_{45} - v_{47} \tag{176}$$

9.30 Species PXRprot_DEX

Name PXRprot_DEX

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

This species takes part in six reactions (as a reactant in re31, re33 and as a product in re30 and as a modifier in re30, re31, re33).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PXRprot\_DEX} = v_{38} - v_{39} - v_{41} \tag{177}$$

9.31 Species DEX_degr

Name DEX_degr

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

This species takes part in one reaction (as a product in re32), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DEX\_degr} = 0 \tag{178}$$

9.32 Species CYPgene_PXRprot_DEX

Name CYPgene_PXRprot_DEX

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

This species takes part in four reactions (as a product in re33 and as a modifier in re33, re34, re34).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CYPgene\_PXRprot\_DEX} = v_{41} \tag{179}$$

9.33 Species PXRgene_GRprot_DEX

Name PXRgene_GRprot_DEX

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

This species takes part in four reactions (as a product in re35 and as a modifier in re35, re36, re36).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PXRgene\_GRprot\_DEX} = v_{43} \tag{180}$$

9.34 Species GRgene_GRprot_DEX

Name GRgene_GRprot_DEX

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

This species takes part in four reactions (as a product in re37 and as a modifier in re37, re38, re38).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GRgene\_GRprot\_DEX} = v_{45} \tag{181}$$

9.35 Species TATgene_GRprot_DEX

Name TATgene_GRprot_DEX

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

This species takes part in four reactions (as a product in re39 and as a modifier in re39, re40, re40).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TATgene\_GRprot\_DEX} = v_{47} \tag{182}$$

9.36 Species s2

Name CortOUT

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

This species takes part in seven reactions (as a reactant in cortisolTransport, Cortisol_CBG, Cort_Alb and as a product in cort_distribution and as a modifier in cortisolTransport, Cortisol_CBG, Cort_Alb).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s2} = v_{52} - v_{31} - v_{50} - v_{51} \tag{183}$$

9.37 Species DEXout

Name DEXout

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

This species takes part in two reactions (as a reactant in re41 and as a modifier in re41), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DEXout} = 0 \tag{184}$$

9.38 Species CBG

Name CBG

Initial concentration $550.000163480092\ \text{nmol} \cdot \text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CBG} = -v_{50} \tag{185}$$

9.39 Species CBG_CortOUT

Name CBG_CortOUT

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

This species takes part in two reactions (as a product in Cortisol_CBG and as a modifier in Cortisol_CBG).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CBG\_CortOUT} = v_{50} \tag{186}$$

9.40 Species Alb

Name Alb

Initial concentration 60000.0178341918 nmol · l^{-1}

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Alb} = -v_{51} \tag{187}$$

9.41 Species Alb_CortOUT

Name Alb_CortOUT

Initial concentration 0 nmol · l^{-1}

This species takes part in two reactions (as a product in Cort_Alb and as a modifier in Cort_Alb).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Alb\_CortOUT} = v_{51} \tag{188}$$

9.42 Species CortAdded

Name CortAdded

Initial concentration 0 nmol · l^{-1}

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CortAdded} = 0 \tag{189}$$

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