

## SBML Model Report

# Model name: “Stavrum2013 - Tryptophan Metabolism in Liver”



May 6, 2016

## 1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following eleven authors: Ryan Gutenkunst<sup>1</sup>, Bao Charles<sup>2</sup>, Gillette Heather<sup>3</sup>, Lichauco Katrina<sup>4</sup>, Valenzuela Piriscilla<sup>5</sup>, Grover Jeffrey<sup>6</sup>, Ahmed Nasiha<sup>7</sup>, Trujillo Joshua<sup>8</sup>, Palazzola Dominic<sup>9</sup>, Ines Heiland<sup>10</sup> and Vijayalakshmi Chelliah<sup>11</sup> at April 18<sup>th</sup> 2016 at 2:06 p. m. and last time modified at April 18<sup>th</sup> 2016 at three o’ clock in the afternoon. Table 1 shows an overview of the quantities of all components of this model.

## Model Notes

This model is from the paper:

Anne-Kristin Stavrum, Ines Heiland, Stefan Schuster, Pl Puntervoll, and Mathias Ziegler.

Summary:

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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	56
events	0	constraints	0
reactions	42	function definitions	0
global parameters	42	unit definitions	1
rules	0	initial assignments	0

Tryptophan is utilised in various metabolic routes including protein synthesis, serotonin

## 2 Unit Definitions

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

### 2.1 Unit substance

**Name** substance

**Definition** mmol

### 2.2 Unit volume

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

**Definition** l

### 2.3 Unit area

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

**Definition** m<sup>2</sup>

### 2.4 Unit length

**Notes** Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

**Definition** m

### 2.5 Unit time

**Notes** Second is the predefined SBML unit for time.

**Definition** s

### 3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
Cytosol	Cytosol		3	1	litre	<input checked="" type="checkbox"/>	

#### 3.1 Compartment Cytosol

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

**Name** Cytosol

## 4 Species

This model contains 56 species. The boundary condition of 42 of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 7 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
M_3hanthrn_c	M_3HAA	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_5hoxfkyn_c	M_5HFKyn	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_5htrp_c	M_5HTrp	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_5hxkyn_c	M_5HKyn	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_Lfmkynr_c	M_FKyn	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_Lkynr_c	M_L-Kyn	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_ahcys_c	M_AHCys	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_akg_c	M_Ketoglutarate	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_ala_DASH_L_c	M_L-ALA	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_amet_c	M-AMet	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_anth_c	M-AA	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_cmusa_c	M-Acms	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_dhbpt_c	M-Dhbpt	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_for_c	M-Formate	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_glu_DASH_L_c	M-LGlu	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_hLkynr_c	M_3HKyn	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_id3acald_c	M-IndolAc	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_indpyr_c	M-IndolP	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_nmtrpta_c	M-MTrypta	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_quln_c	M-Quin	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_srtln_c	M-Serotonin	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
M_thbpt	M_Thbpt	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_trna_trp_c	M_tRNA	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_trp_DASH_L_c	M_Trp	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_trp_L_trna_c	M_Trp_tRNA	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_trypta_c	M_Trypta	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_amp_c	M_AMP	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_atp_c	M_ATP	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_co2_c	M_CO2	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_h2o2_c	M_H2O2	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_h2o_c	M_H2O	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_h_c	M_H	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_nadp_c	M_NADP	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_nadph_c	M_NADPH	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_nh4_c	M_NH4	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_o2_c	M_O2	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_o2s_c	M_O2s	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_ppi_c	M_PPi	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M- _Cinnavalininate_c	M_Cin	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_kynate_c	M_Kyna	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
TRP_ex	Trp_ex	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_nicrnt_c	M_NaMN	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_prpp_c	M_PRPP	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_nformanth_c	M_FAA	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
M_dnad_c	M_NAAD	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_am6sa_c	M_Am6sa	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_5hoxindact_c	M_5HAc	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
M_Nacsertn_c	M_NAcSet	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_accoa_c	M_AcetylCoA	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_coa_c	M_CoA	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_Xanthurenate	M_Xanth	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_f5hoxkyn_c	M_F5HKyn	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_nndmtrpta_c	M_MMTrypta	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_nmsrtn_c	M_NMSer	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_Nactrypta_c	M_Nactrypta	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
M_Lkynr_ex	M_LKyn_ex	Cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

## 5 Parameters

This model contains 42 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
scaling	scaling		1.000		✓
AADAT_E_T- _kat1	KAT1_E_T		9455.136		✓
AADAT_E_T- _kat2	KAT2_E_T		7744.315		✓
AADAT_E_T- _kat3	KAT3_E_T		15588.210		✓
AADAT_Km- _hLkynr	KAT_Km_3HKyn		3.800		✓
AADAT_Km- _Lkynr	KAT_Km_L-kyn		4.700		✓
AANAT_E_T	AANAT_E_T		2770.968		✓
AANAT_Km- _Srtn	AANAT_Km- _Serotonin		1.350		✓
AANAT_Km- _trypta	AANAT_Km- _Trypta		0.880		✓
AFMID_E_T	AFMID_E_T		15820.216		✓
AFMID_Km- _5hoxnfky	AFMID_Km- _5HFKyn		0.400		✓
AFMID_Km- _Lfmkynr	AFMID_Km_FKyn		0.050		✓
AFMID_Km- _nformanth	AFMID_Km_FAA		0.211		✓
DDC_E_T	DDC_E_T		36074.914		✓
DDC_Km_5htrp	DDC_Km_5htrp		0.049		✓
DDC_Km_trp- _DASH_L	DDC_Km_Trp		10.000		✓
IDO_E_T	IDO_E_T		453.483		✓
IDO_Km_trp- _DASH_L	IDO_Km_Trp		0.045		✓
IDO_Km_5htrp	IDO_Km_5htrp		0.020		✓
IDO_Km_srtn	IDO_Km- _Serotonin		0.100		✓
IMNT_E_T	IMNT_E_T		4186.587		✓
IMNT_Km_srtn	IMNT_Km- _Serotonin		1.380		✓

Id	Name	SBO	Value	Unit	Constant
IMNT_Km-_trypta	IMNT_Km_Trypta		0.270		✓
IMNT_Km-_nmtrpta	IMNT_Km-_MTrypta		0.086		✓
KYNU_Km-_hLkynr	KYNU_Km-_3HKyn		0.028		✓
Transporter-_E_T_Slc7a8	Transporter_E_T-_Slc7a8		2226.373		✓
KYNU_E_T	KYNU_E_T		56601.758		✓
KYNU_Km-_Lfmkynr	KYNU_Km_FKyn		2.200		✓
KYNU_Km-_Lkynr	KYNU_Km_L-kyn		0.495		✓
Transporter-_Km_Lkynr	Transporter_Km_L-kyn		0.032		✓
Transporter-_Km_Trp-_Slc7a8	Transporter_Km-_Trp_Slc7a8		0.057		✓
Transporter-_E_T_Slc7a5	Transporter_E_T-_Slc7a5		1961.514		✓
Transporter-_Km_Trp-_Slc7a5	Transporter_Km-_Trp_Slc7a5		0.019		✓
MAOA_E_T	MAOA_E_T		137204.813		✓
MAOB_E_T	MAOB_E_T		294114.875		✓
MAO_Km_srttn	MAO_Km-_Serotonin		0.430		✓
MAO_Km-_trypta	MAO_Km_Trypta		0.033		✓
IDO_Km_O2	IDO_Km_O2		0.042		✓
AADAT_kcat-_hLkynr	KAT_kcat_3HKyn		1.700		✓
AADAT_kcat-_Lkynr	KAT_kcat_L-kyn		9.760		✓
Transporter-_kcat_Trp	Transporter_kcat-_Trp		1.300		✓
Transporter-_kcat_Lkynr	Transporter_kcat-_L-kyn		1.300		✓



## 6 Reactions

This model contains 42 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

Nº	Id	Name	Reaction Equation	SBO
1	R00677	IL4I1	$\text{M\_trp\_DASH\_L\_c} + \text{M\_h2o\_c} + \text{M\_o2\_c} \xrightarrow{\text{M\_h2o\_c}, \text{M\_o2\_c}, \text{M\_trp\_DASH\_L\_c}} \text{M\_indpyr\_c} + \text{M\_nh4\_c} + \text{M\_h2o2\_c}$	
2	R00678_Tdo	TDO	$\text{M\_trp\_DASH\_L\_c} + \text{M\_o2\_c} \xrightarrow{\text{M\_o2\_c}, \text{M\_trp\_DASH\_L\_c}} \text{M\_Lfmkynr\_c}$	
3	R00685	DDC_Trypta	$\text{M\_trp\_DASH\_L\_c} \xrightarrow{\text{M\_5htrp\_c}, \text{M\_trp\_DASH\_L\_c}} \text{M\_trypta\_c} + \text{M\_co2\_c}$	
4	R00987	KYNU_L-Kyn	$\text{M\_Lkynr\_c} + \text{M\_h2o\_c} \xrightarrow{\text{M\_hLkynr\_c}, \text{M\_Lfmkynr\_c}, \text{M\_Lkynr\_c}} \text{M\_anth\_c} + \text{M\_ala\_DASH\_L\_c}$	
5	R01814_Tph1	TPH1	$\text{M\_thbpt} + \text{M\_trp\_DASH\_L\_c} + \text{M\_o2\_c} \xrightarrow{\text{M\_o2\_c}, \text{M\_thbpt}, \text{M\_trp\_DASH\_L\_c}} \text{M\_5htrp\_c} + \text{M\_dhbpt\_c} + \text{M\_h2o\_c}$	
6	R01956_Kat1	KAT1_L-Kyn	$\text{M\_Lkynr\_c} + \text{M\_akg\_c} \xrightarrow{\text{M\_hLkynr\_c}, \text{M\_Lkynr\_c}} \text{M\_kynate\_c} + \text{M\_glu\_DASH\_L\_c}$	
7	R01959	AFMID.FKyn	$\text{M\_Lfmkynr\_c} + \text{M\_h2o\_c} \xrightarrow{\text{M\_5hoxnfkyn\_c}, \text{M\_nformanth\_c}, \text{M\_Lfmkynr\_c}} \text{M\_for\_c} + \text{M\_Lkynr\_c}$	
8	R01960	KMO	$\text{M\_Lkynr\_c} + \text{M\_o2\_c} + \text{M\_nadph\_c} + \text{M\_h\_c} \xrightarrow{\text{M\_Lkynr\_c}, \text{M\_h\_c}, \text{M\_nadph\_c}, \text{M\_o2\_c}} \text{M\_hLkynr\_c} + \text{M\_nadp\_c} + \text{M\_h2o\_c}$	

Nº	Id	Name	Reaction Equation	SBO
9	R02174	INMT_Trypta	$\text{M\_amet\_c} + \text{M\_trypta\_c} \xrightarrow{\text{M\_nmtrpta\_c}, \text{M\_srt\_c}, \text{M\_trypta\_c}} \text{M\_ahcys\_c} + \text{M\_nmtrpta\_c}$	
10	R02665	HAAO	$\text{M\_3hanthrn\_c} + \text{M\_o2\_c} \xrightarrow{\text{M\_quln\_c}, \text{M\_anth\_c}, \text{M\_3hanthrn\_c}, \text{M\_o2\_c}} \text{M\_cmusa\_c}$	
11	R02668	KYNU_3HKyn	$\text{M\_hLkynr\_c} + \text{M\_h2o\_c} \xrightarrow{\text{M\_Lkynr\_c}, \text{M\_Lfmkynr\_c}, \text{M\_hLkynr\_c}} \text{M\_3hanthrn\_c} + \text{M\_ala\_DASH\_L\_c}$	
12	R02701	DDC_5HTrp	$\text{M\_5htrp\_c} \xrightarrow{\text{M\_trp\_DASH\_L\_c}, \text{M\_5htrp\_c}} \text{M\_srt\_c} + \text{M\_co2\_c}$	
13	R02702	IDO_5HTrp	$\text{M\_5htrp\_c} + \text{M\_o2\_c} \xrightarrow{\text{M\_trp\_DASH\_L\_c}, \text{M\_srt\_c}, \text{M\_5htrp\_c}, \text{M\_o2\_c}} \text{M\_5hoxnfkyn\_c}$	
14	R03664	WARS	$\begin{aligned} &\text{M\_atp\_c} + \text{M\_trp\_DASH\_L\_c} + \\ &\text{M\_trna\_trp\_c} \xrightarrow{\text{M\_atp\_c}, \text{M\_trna\_trp\_c}, \text{M\_trp\_DASH\_L\_c}} \text{M\_amp\_c} + \\ &\text{M\_ppi\_c} + \text{M\_trp\_L\_trna\_c} \end{aligned}$	
15	R04911	AFMID_5HFKyn	$\text{M\_5hoxnfkyn\_c} + \text{M\_h2o\_c} \xrightarrow{\text{M\_Lfmkynr\_c}, \text{M\_nformanth\_c}, \text{M\_5hoxnfkyn\_c}} \text{M\_5hxkyn} + \text{M\_for\_c}$	
16	quin_form	Quinolic Acid formation (spontaneous)	$\text{M\_cmusa\_c} \xrightarrow{\text{M\_cmusa\_c}} \text{M\_quln\_c}$	
17	R02173_Maoa	MAOA_Trypta	$\begin{aligned} &\text{M\_trypta\_c} + \text{M\_h2o\_c} + \\ &\text{M\_o2\_c} \xrightarrow{\text{M\_srt\_c}, \text{M\_trypta\_c}} \text{M\_id3acald\_c} + \\ &\text{M\_nh4\_c} + \text{M\_h2o2\_c} \end{aligned}$	
18	R02670	Cinnavalinate formation	$\begin{aligned} &2 \text{M\_3hanthrn\_c} + 4 \text{M\_o2\_c} \xrightarrow{\text{M\_3hanthrn\_c}, \text{M\_o2\_c}} \text{M\_Cinnavalinate\_c} + \\ &2 \text{M\_o2s\_c} + 2 \text{M\_h2o2\_c} + 2 \text{M\_h\_c} \end{aligned}$	
19	TRPtrans_Slc7a5	Tryptophan_Transport Slc7a5	$\text{TRP\_ex} \xrightarrow{\text{M\_Lkynr\_ex}, \text{M\_Lkynr\_c}, \text{M\_trp\_DASH\_L\_c}, \text{TRP\_ex}} \text{M\_trp\_DASH\_L\_c}$	
20	R00678_Indo	IDO	$\begin{aligned} &\text{M\_trp\_DASH\_L\_c} + \\ &\text{M\_o2\_c} \xrightarrow{\text{M\_5htrp\_c}, \text{M\_srt\_c}, \text{M\_o2\_c}, \text{M\_trp\_DASH\_L\_c}} \text{M\_Lfmkynr\_c} \end{aligned}$	

Nº	Id	Name	Reaction Equation	SBO
21	R03348	QPRT	$\begin{aligned} & \text{M\_h\_c} + \text{M\_prpp\_c} + \\ & \text{M\_quln\_c} \xrightarrow{\text{M\_h\_c}, \text{M\_prpp\_c}, \text{M\_quln\_c}} \text{M\_co2\_c} + \\ & \text{M\_nicrnt\_c} + \text{M\_ppi\_c} \end{aligned}$	
22	R03936	KYNU_FKyn	$\text{M\_Lfmkynr\_c} + \text{M\_h2o\_c} \xrightarrow{\text{M\_Lkynr\_c}, \text{M\_hLkynr\_c}, \text{M\_Lfmkynr\_c}} \text{M\_nformanth\_c} + \text{M\_ala\_DASH\_L\_c}$	
23	R00988	AFMID_FAA	$\text{M\_nformanth\_c} + \text{M\_h2o\_c} \xrightarrow{\text{M\_Lfmkynr\_c}, \text{M\_5hoxnfkyn\_c}, \text{M\_nformanth\_c}} \text{M\_for\_c} + \text{M\_anth\_c}$	
24	R03005	NMNAT1	$\begin{aligned} & \text{M\_atp\_c} + \text{M\_h\_c} + \\ & \text{M\_nicrnt\_c} \xrightarrow{\text{M\_atp\_c}, \text{M\_h\_c}, \text{M\_nicrnt\_c}} \text{M\_dnad\_c} + \\ & \text{M\_ppi\_c} \end{aligned}$	
25	R04323	ACMSD	$\text{M\_cmusa\_c} \xrightarrow{\text{M\_quln\_c}, \text{M\_kynate\_c}, \text{M\_cmusa\_c}} \text{M\_am6sa\_c} + \text{M\_co2\_c}$	
26	R02908_Maoa	MAOA_Serotonin	$\begin{aligned} & \text{M\_srt n\_c} + \text{M\_h2o\_c} + \\ & \text{M\_o2\_c} \xrightarrow{\text{M\_trypta\_c}, \text{M\_5hxkyn\_c}, \text{M\_srt n\_c}} \text{M\_5hoxindact\_c} + \\ & \text{M\_h2o2\_c} + \text{M\_nh4\_c} \end{aligned}$	
27	R02911	AANAT_Serotonin	$\begin{aligned} & \text{M\_accoa\_c} + \text{M\_srt n\_c} \xrightarrow{\text{M\_trypta\_c}, \text{M\_srt n\_c}} \text{M\_Nacsert n\_c} + \\ & \text{M\_coa\_c} + \text{M\_h\_c} \end{aligned}$	
28	R04171_Kat1	KAT1_3HKyn	$\begin{aligned} & \text{M\_hLkynr\_c} + \text{M\_akg\_c} \xrightarrow{\text{M\_Lkynr\_c}, \text{M\_hLkynr\_c}} \text{M\_Xanthurenate} + \\ & \text{M\_glu\_DASH\_L\_c} \end{aligned}$	
29	R02909	IDO_Serotonin	$\text{M\_srt n\_c} + \text{M\_o2\_c} \xrightarrow{\text{M\_5htrp\_c}, \text{M\_trp\_DASH\_L\_c}, \text{M\_o2\_c}, \text{M\_srt n\_c}} \text{M\_f5hoxkyn\_c}$	
30	R02174- _metTrypta	INMT_MTrypta	$\begin{aligned} & \text{M\_amet\_c} + \text{M\_nmtrpta\_c} \xrightarrow{\text{M\_srt n\_c}, \text{M\_trypta\_c}, \text{M\_nmtrpta\_c}} \text{M\_ahcys\_c} + \\ & \text{M\_nndmtrpta\_c} \end{aligned}$	
31	R02910	INMT_Serotonin	$\begin{aligned} & \text{M\_amet\_c} + \text{M\_srt n\_c} \xrightarrow{\text{M\_nmtrpta\_c}, \text{M\_trypta\_c}, \text{M\_srt n\_c}} \text{M\_ahcys\_c} + \\ & \text{M\_nmsrt n\_c} \end{aligned}$	

Nº	Id	Name	Reaction Equation	SBO
32	R01956_Kat2	KAT2_3HKyn	$\text{M\_hLkynr\_c} + \text{M\_akg\_c} \xrightarrow{\text{M\_Lkynr\_c}, \text{M\_hLkynr\_c}} \text{M\_Xanthurenate} + \text{M\_glu\_DASH\_L\_c}$	
33	R01956_Kat3	KAT3_3HKyn	$\text{M\_hLkynr\_c} + \text{M\_akg\_c} \xrightarrow{\text{M\_Lkynr\_c}, \text{M\_hLkynr\_c}} \text{M\_Xanthurenate} + \text{M\_glu\_DASH\_L\_c}$	
34	R04171_Kat2	KAT2_L-Kyn	$\text{M\_Lkynr\_c} + \text{M\_akg\_c} \xrightarrow{\text{M\_hLkynr\_c}, \text{M\_Lkynr\_c}} \text{M\_kynate\_c} + \text{M\_glu\_DASH\_L\_c}$	
35	R04171_Kat3	KAT3_L-Kyn	$\text{M\_Lkynr\_c} + \text{M\_akg\_c} \xrightarrow{\text{M\_hLkynr\_c}, \text{M\_Lkynr\_c}} \text{M\_kynate\_c} + \text{M\_glu\_DASH\_L\_c}$	
36	R02908_Maob	MAOB_Serotonin	$\text{M\_srtm\_c} + \text{M\_h2o\_c} \xrightarrow{\text{M\_trypta\_c}, \text{M\_5hxykn\_c}, \text{M\_srtm\_c}} \text{M\_5hoxindact\_c} + \text{M\_h2o2\_c} + \text{M\_nh4\_c}$	
37	R02173_Maob	MAOB_Trypta	$\text{M\_trypta\_c} + \text{M\_h2o\_c} \xrightarrow{\text{M\_srtm\_c}, \text{M\_trypta\_c}} \text{M\_id3acald\_c} + \text{M\_nh4\_c} + \text{M\_h2o2\_c}$	
38	AANAT_Trypta	AANAT_Trypta	$\text{M\_accoa\_c} + \text{M\_trypta\_c} \xrightarrow{\text{M\_srtm\_c}, \text{M\_trypta\_c}} \text{M\_Nactrypta\_c} + \text{M\_coa\_c} + \text{M\_h\_c}$	
39	R01814_Tph2	TPH2	$\text{M\_thbpt} + \text{M\_trp\_DASH\_L\_c} \xrightarrow{\text{M\_o2\_c}, \text{M\_thbpt}, \text{M\_trp\_DASH\_L\_c}} \text{M\_5htrp\_c} + \text{M\_dhbpt\_c} + \text{M\_h2o\_c}$	
40	TRPtrans_Slc7a8	Tryptophan_Transport_Slc7a8	$\text{TRP\_ex} \xrightleftharpoons{\text{M\_Lkynr\_ex}, \text{M\_Lkynr\_c}, \text{M\_trp\_DASH\_L\_c}, \text{TRP\_ex}} \text{M\_trp\_DASH\_L\_c}$	
41	Lkynr_trans-Slc7a5	Lkynr_Transporter_Slc7a5	$\text{M\_Lkynr\_c} \xrightleftharpoons{\text{M\_trp\_DASH\_L\_c}, \text{TRP\_ex}, \text{M\_Lkynr\_c}, \text{M\_Lkynr\_ex}} \text{M\_Lkynr\_ex}$	
42	Lkynr_trans-Slc7a8	Lkynr_Transporter_Slc7a8	$\text{M\_Lkynr\_c} \xrightleftharpoons{\text{M\_trp\_DASH\_L\_c}, \text{TRP\_ex}, \text{M\_Lkynr\_c}, \text{M\_Lkynr\_ex}} \text{M\_Lkynr\_ex}$	

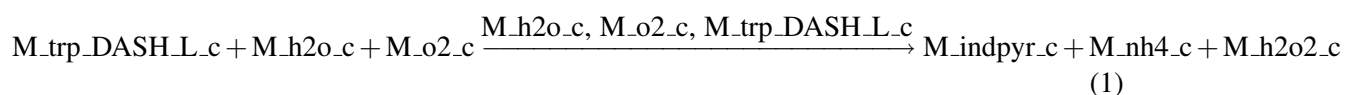
Nº	Id	Name	Reaction Equation	SBO
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## 6.1 Reaction R00677

This is an irreversible reaction of three reactants forming three products influenced by three modifiers.

**Name** IL4I1

### Reaction equation



### Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
M_trp_DASH_L_c	M_Trp	
M_h2o_c	M_H2O	
M_o2_c	M_O2	

### Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
M_h2o_c	M_H2O	
M_o2_c	M_O2	
M_trp_DASH_L_c	M_Trp	

### Products

Table 8: Properties of each product.

Id	Name	SBO
M_indpyr_c	M_IndolP	
M_nh4_c	M_NH4	
M_h2o2_c	M_H2O2	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_1 = \text{vol}(\text{Cytosol}) \cdot \frac{k_{\text{cat}} \cdot E_T \cdot [M_{\text{trp\_DASH\_L\_c}}] \cdot [M_{\text{o2\_c}}] \cdot [M_{\text{h2o\_c}}] \cdot \text{scaling}}{K_a \cdot K_b + K_b \cdot [M_{\text{trp\_DASH\_L\_c}}] + K_a \cdot [M_{\text{o2\_c}}] + [M_{\text{trp\_DASH\_L\_c}}] \cdot [M_{\text{o2\_c}}]} \quad (2)$$

Table 9: Properties of each parameter.

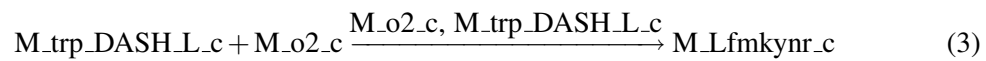
Id	Name	SBO	Value	Unit	Constant
E_T	E_T		2046.74		<input checked="" type="checkbox"/>
Ka	Ka		6.50		<input checked="" type="checkbox"/>
Kb	Kb		1.20		<input checked="" type="checkbox"/>
kcat	kcat		1.00		<input checked="" type="checkbox"/>

## 6.2 Reaction R00678\_Tdo

This is an irreversible reaction of two reactants forming one product influenced by two modifiers.

**Name** TDO

### Reaction equation



### Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
M_trp_DASH_L_c	M_Trp	
M_o2_c	M_O2	

### Modifiers

Table 11: Properties of each modifier.

Id	Name	SBO
M_o2_c	M_O2	
M_trp_DASH_L_c	M_Trp	

### Product

Table 12: Properties of each product.

Id	Name	SBO
M_Lfmkynr_c	M_FKyn	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_2 = \text{vol}(\text{Cytosol}) \cdot \frac{\text{kcat} \cdot E\_T \cdot [M\_trp\_DASH\_L\_c] \cdot [M\_o2\_c] \cdot \text{scaling}}{K_a \cdot K_b + K_a \cdot [M\_o2\_c] + K_b \cdot [M\_trp\_DASH\_L\_c] + [M\_trp\_DASH\_L\_c] \cdot [M\_o2\_c]} \quad (4)$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
E_T	E_T		943912.000		✓
Ka	Ka		0.222		✓
Kb	Kb		0.037		✓
kcat	kcat		1.400		✓

### 6.3 Reaction R00685

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

**Name** DDC\_Trypta

**Notes** km and kcat values taken from 4991409 (pig)

### Reaction equation



### Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
M_trp_DASH_L_c	M_Trp	



## Modifiers

Table 15: Properties of each modifier.

Id	Name	SBO
M_5htrp_c	M_5HTrp	
M_trp_DASH_L_c	M_Trp	

## Products

Table 16: Properties of each product.

Id	Name	SBO
M_trypta_c	M_Trypta	
M_co2_c	M_CO2	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_3 = \text{vol}(\text{Cytosol}) \cdot \frac{\text{DDC\_E\_T} \cdot \text{kat\_B} \cdot \text{scaling} \cdot [\text{M\_trp\_DASH\_L\_c}] \cdot \text{DDC\_Km\_5htrp}}{\text{DDC\_Km\_trp\_DASH\_L} \cdot \text{DDC\_Km\_5htrp} + \text{DDC\_Km\_trp\_DASH\_L} \cdot [\text{M\_5htrp\_c}] + \text{DDC\_Km\_5htrp} \cdot [\text{M\_trp\_DASH\_L\_c}]} \quad (6)$$

Table 17: Properties of each parameter.

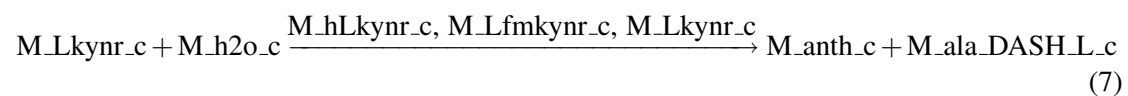
Id	Name	SBO	Value	Unit	Constant
kat_B	kat_B		0.38		<input checked="" type="checkbox"/>

## 6.4 Reaction R00987

This is an irreversible reaction of two reactants forming two products influenced by three modifiers.

**Name** KYNU\_L-Kyn

### Reaction equation



## Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
M_Lkynr_c	M_L-Kyn	
M_h2o_c	M_H2O	

## Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
M_hLkynr_c	M_3HKyn	
M_Lfmkynr_c	M_FKyn	
M_Lkynr_c	M_L-Kyn	

## Products

Table 20: Properties of each product.

Id	Name	SBO
M_anth_c	M_AA	
M_mla_DASH_L_c	M_LALA	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_4 = \text{vol}(\text{Cytosol}) \cdot \frac{\text{KYNU\_E\_T} \cdot \text{kcat\_A} \cdot \text{scaling} \cdot [\text{M}]}{\text{KYNU\_Km\_Lkynr} \cdot \text{KYNU\_Km\_hLkynr} \cdot \text{KYNU\_Km\_Lfmkynr} + \text{KYNU\_Km\_hLkynr} \cdot \text{KYNU\_Km\_Lfmkynr}} \quad (8)$$

Table 21: Properties of each parameter.

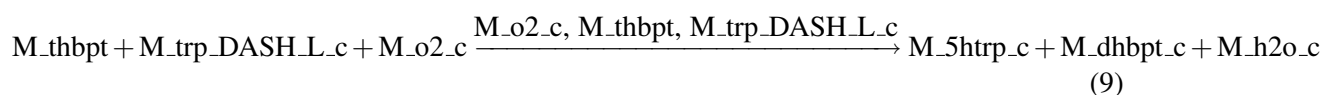
Id	Name	SBO	Value	Unit	Constant
kcat_A	kcat_A		0.23		<input checked="" type="checkbox"/>

## 6.5 Reaction R01814\_Tph1

This is an irreversible reaction of three reactants forming three products influenced by three modifiers.

**Name** TPH1

### Reaction equation



### Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
M_thbpt	M_Thbpt	
M_trp_DASH_L_c	M_Trp	
M_o2_c	M_O2	

### Modifiers

Table 23: Properties of each modifier.

Id	Name	SBO
M_o2_c	M_O2	
M_thbpt	M_Thbpt	
M_trp_DASH_L_c	M_Trp	

### Products

Table 24: Properties of each product.

Id	Name	SBO
M_5htrp_c	M_5HTrp	
M_dhhbpt_c	M_Dhbpt	
M_h2o_c	M_H2O	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_5 = \text{vol}(\text{Cytosol}) \cdot \frac{\text{kcat} \cdot E\_T \cdot [M\_trp\_DASH\_L\_c] \cdot [M\_o2\_c] \cdot [M\_thbpt] \cdot \text{scaling}}{K_a \cdot K_b + K_b \cdot [M\_trp\_DASH\_L\_c] + K_a \cdot [M\_o2\_c] + [M\_trp\_DASH\_L\_c] \cdot [M\_o2\_c]} \quad (10)$$

Table 25: Properties of each parameter.

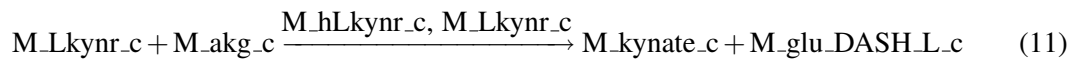
Id	Name	SBO	Value	Unit	Constant
E_T	E_T		503.141		✓
Ka	Ka		0.023		✓
Kb	Kb		0.109		✓
kcat	kcat		0.570		✓

## 6.6 Reaction R01956\_Kat1

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

**Name** KAT1\_L-Kyn

### Reaction equation



### Reactants

Table 26: Properties of each reactant.

Id	Name	SBO
M_Lkynr_c	M.L-Kyn	
M_akg_c	M.Ketoglutarate	

### Modifiers

Table 27: Properties of each modifier.

Id	Name	SBO
M_hLkynr_c	M.3HKyn	
M_Lkynr_c	M.L-Kyn	

## Products

Table 28: Properties of each product.

Id	Name	SBO
M_kynate_c	M_Kyna	
M_glu_DASH_L_c	M_LGlu	

## Kinetic Law

**Derived unit** contains undeclared units

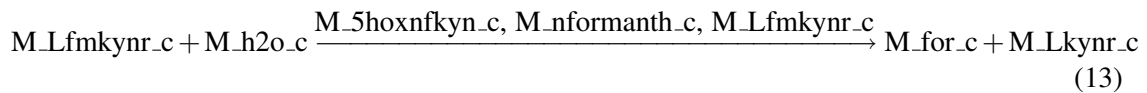
$$v_6 = \text{vol}(\text{Cytosol}) \cdot \frac{\text{AADAT\_E\_T\_kat1} \cdot \text{AADAT\_kcat\_Lkynr} \cdot \text{scaling} \cdot [\text{M\_Lkynr\_c}] \cdot \text{AADAT\_Km\_hLkynr}}{\text{AADAT\_Km\_Lkynr} \cdot \text{AADAT\_Km\_hLkynr} + \text{AADAT\_Km\_Lkynr} \cdot [\text{M\_hLkynr\_c}] + \text{AADAT\_Km\_hLkynr} \cdot [\text{M\_Lkynr\_c}]} \quad (12)$$

## 6.7 Reaction R01959

This is an irreversible reaction of two reactants forming two products influenced by three modifiers.

**Name** AFMID\_FKyn

## Reaction equation



## Reactants

Table 29: Properties of each reactant.

Id	Name	SBO
M_Lfmkynr_c	M_FKyn	
M_h2o_c	M_H2O	

## Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
M_5hoxnfkyn_c	M_5HFKyn	

Id	Name	SBO
M_nformanth_c	M_FAA	
M_Lfmkynr_c	M_FKyn	

### Products

Table 31: Properties of each product.

Id	Name	SBO
M_for_c	M.Formate	
M_Lkynr_c	M_L-Kyn	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_7 = \text{vol}(\text{Cytosol}) \cdot \frac{\text{AFMID\_E\_T} \cdot \text{kcat\_A}}{\text{AFMID\_Km\_Lfmkynr} \cdot \text{AFMID\_Km\_5hoxnfky} \cdot \text{AFMID\_Km\_nformanth} + \text{AFMID\_Km\_5hoxnfky} \cdot \text{AFMID\_Km\_Lkynr} + \text{AFMID\_Km\_Lfmkynr} \cdot \text{AFMID\_Km\_5hoxnfky}} \quad (14)$$

Table 32: Properties of each parameter.

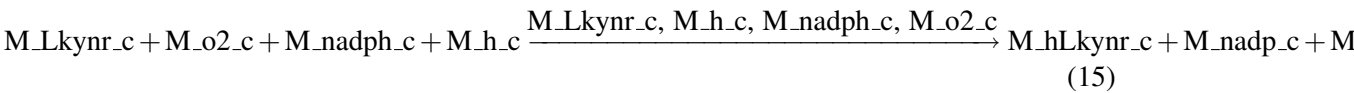
Id	Name	SBO	Value	Unit	Constant
kcat_A	kcat_A		100.0		<input checked="" type="checkbox"/>

### 6.8 Reaction R01960

This is an irreversible reaction of four reactants forming three products influenced by four modifiers.

**Name** KMO

### Reaction equation



### Reactants

Table 33: Properties of each reactant.

Id	Name	SBO
M_Lkynr_c	M.L-Kyn	
M_o2_c	M.O2	
M_nadph_c	M.NADPH	
M_h_c	M.H	

## Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
M_Lkynr_c	M.L-Kyn	
M_h_c	M.H	
M_nadph_c	M.NADPH	
M_o2_c	M.O2	

## Products

Table 35: Properties of each product.

Id	Name	SBO
M_hLkynr_c	M.3HKyn	
M_nadp_c	M.NADP	
M_h2o_c	M.H2O	

## Kinetic Law

**Derived unit** contains undeclared units

$v_8 = \text{vol}(\text{Cytosol})$

$$v_8 = \frac{\text{kcat} \cdot E\_T \cdot [M\_Lkynr\_c] \cdot [M\_o2\_c]}{K_a \cdot K_b \cdot K_c + [M\_Lkynr\_c] \cdot K_b \cdot K_c + [M\_o2\_c] \cdot K_a \cdot K_c + [M\_nadph\_c] \cdot K_a \cdot K_b + [M\_Lkynr\_c] \cdot [M\_o2\_c]}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
E_T	E_T		9766.180		✓
Ka	Ka		0.100		✓

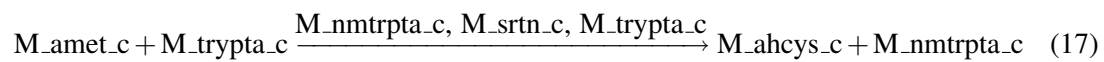
Id	Name	SBO	Value	Unit	Constant
Kb	Kb		0.071		<input checked="" type="checkbox"/>
Kc	Kc		0.153		<input checked="" type="checkbox"/>
kcat	kcat		2.200		<input checked="" type="checkbox"/>

## 6.9 Reaction R02174

This is an irreversible reaction of two reactants forming two products influenced by three modifiers.

**Name** INMT\_Trypta

### Reaction equation



### Reactants

Table 37: Properties of each reactant.

Id	Name	SBO
M_amet_c	M_AMet	
M_trypta_c	M_Trypta	

### Modifiers

Table 38: Properties of each modifier.

Id	Name	SBO
M_nmtrpta_c	M_MTrypta	
M_srt n_c	M_Serotonin	
M_trypta_c	M_Trypta	

### Products

Table 39: Properties of each product.

Id	Name	SBO
M_ahcys_c	M_AHCys	
M_nmtrpta_c	M_MTrypta	



## Kinetic Law

**Derived unit** contains undeclared units

$$v_9 = \text{vol}(\text{Cytosol}) \cdot \frac{\text{IMNT\_E\_T} \cdot \text{kcat\_A} \cdot \text{scaling} \cdot [\text{M\_trypta\_c}]}{\text{IMNT\_Km\_trypta} \cdot \text{IMNT\_Km\_nmtrpta} \cdot \text{IMNT\_Km\_srtn} + \text{IMNT\_Km\_nmtrpta} \cdot \text{IMNT\_Km\_srtn} \cdot [\text{M\_trypta\_c}]} \quad (18)$$

Table 40: Properties of each parameter.

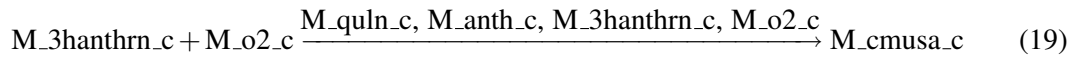
Id	Name	SBO	Value	Unit	Constant
kcat_A	kcat_A		0.4		<input checked="" type="checkbox"/>

## 6.10 Reaction R02665

This is an irreversible reaction of two reactants forming one product influenced by four modifiers.

**Name** HAAO

### Reaction equation



### Reactants

Table 41: Properties of each reactant.

Id	Name	SBO
M_3hanthrn_c	M_3HAA	
M_o2_c	M_O2	

### Modifiers

Table 42: Properties of each modifier.

Id	Name	SBO
M_quln_c	M_Quin	
M_anth_c	M_AA	
M_3hanthrn_c	M_3HAA	
M_o2_c	M_O2	

## Product

Table 43: Properties of each product.

Id	Name	SBO
M_cmusa_c	M_Acms	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{10} = \text{vol}(\text{Cytosol}) \cdot \frac{k_{\text{cat}} \cdot E\_T \cdot [M\_3\text{hanthrn\_c}] \cdot [M\_o2\_c] \cdot \text{scaling}}{K_a \cdot K_b + K_a \cdot [M\_o2\_c] + K_b \cdot [M\_3\text{hanthrn\_c}] + [M\_3\text{hanthrn\_c}] \cdot [M\_o2\_c]} \quad (20)$$

Table 44: Properties of each parameter.

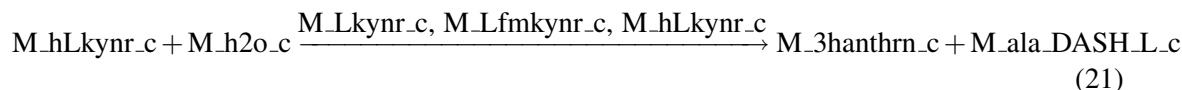
Id	Name	SBO	Value	Unit	Constant
E_T	E_T		10308.400		✓
Ka	Ka		0.016		✓
Kb	Kb		0.615		✓
kcat	kcat		64.000		✓

### 6.11 Reaction R02668

This is an irreversible reaction of two reactants forming two products influenced by three modifiers.

**Name** KYNU\_3HKyn

#### Reaction equation



## Reactants

Table 45: Properties of each reactant.

Id	Name	SBO
M_hLkynr_c	M_3HKyn	
M_h2o_c	M_H2O	

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
M_Lkynr_c	M_L-Kyn	
M_Lfmkynr_c	M_FKyn	
M_hLkynr_c	M_3HKyn	

Products

Table 47: Properties of each product.

Id	Name	SBO
M_3hanthrn_c	M_3HAA	
M_ala_DASH_L_c	M_L_ALA	

Kinetic Law

**Derived unit** contains undeclared units

$$v_{11} = \text{vol}(\text{Cytosol})$$

$$\frac{\text{KYN} \cdot \text{U} \cdot \text{E} \cdot \text{T} \cdot \text{kcat} \cdot \text{A} \cdot \text{scaling} \cdot [\text{M}]}{\text{KYN} \cdot \text{U} \cdot \text{Km} \cdot \text{hLkynr} \cdot \text{KYN} \cdot \text{U} \cdot \text{Km} \cdot \text{Lkynr} \cdot \text{KYN} \cdot \text{U} \cdot \text{Km} \cdot \text{Lfmkynr} + \text{KYN} \cdot \text{U} \cdot \text{Km} \cdot \text{Lkynr} \cdot \text{KYN} \cdot \text{U} \cdot \text{Km} \cdot \text{Lfmkynr} \cdot [\text{M}]}$$

(22)

Table 48: Properties of each parameter.

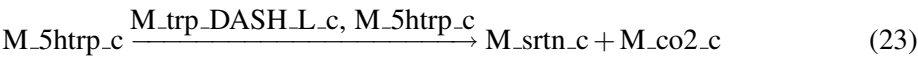
Id	Name	SBO	Value	Unit	Constant
kcat_A	kcat_A		3.5		<input checked="" type="checkbox"/>

6.12 Reaction R02701

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

**Name** DDC\_5HTrp

Reaction equation



## Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
M_5htrp_c	M_5HTrp	

## Modifiers

Table 50: Properties of each modifier.

Id	Name	SBO
M_trp_DASH.L_c	M_Trp	
M_5htrp_c	M_5HTrp	

## Products

Table 51: Properties of each product.

Id	Name	SBO
M_srtm_c	M_Serotonin	
M_co2_c	M.CO2	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{12} = \text{vol}(\text{Cytosol}) \quad (24)$$

$$\frac{\text{DDC\_E\_T} \cdot \text{kcat\_B} \cdot \text{scaling} \cdot [\text{M\_5htrp\_c}] \cdot \text{DDC\_Km\_trp\_DASH.L}}{\text{DDC\_Km\_5htrp} \cdot \text{DDC\_Km\_trp\_DASH.L} + \text{DDC\_Km\_5htrp} \cdot [\text{M\_trp\_DASH.L.c}] + \text{DDC\_Km\_trp\_DASH.L} \cdot [\text{M\_5htrp\_c}]}$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat_B	kcat_B		2.0		<input checked="" type="checkbox"/>

### 6.13 Reaction R02702

This is an irreversible reaction of two reactants forming one product influenced by four modifiers.

**Name** IDO\_5HTrp

### Reaction equation



### Reactants

Table 53: Properties of each reactant.

Id	Name	SBO
M_5htrp_c	M_5HTrp	
M_o2_c	M_O2	

### Modifiers

Table 54: Properties of each modifier.

Id	Name	SBO
M_trp_DASH_L_c	M_Trp	
M_srt_c	M_Serotonin	
M_5htrp_c	M_5HTrp	
M_o2_c	M_O2	

### Product

Table 55: Properties of each product.

Id	Name	SBO
M_5hoxnfkyn_c	M_5HFKyn	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{13} = \text{vol}(\text{Cytosol}) \quad (26)$$

$$\frac{1}{\text{IDO\_Km\_5htrp} \cdot \text{IDO\_Km\_O2} \cdot \text{IDO\_Km\_trp\_DASH\_L} \cdot \text{IDO\_Km\_srt} + [\text{M\_5htrp\_c}] \cdot \text{IDO\_Km\_O2} \cdot \text{IDO\_Km\_L}}$$

Table 56: Properties of each parameter.

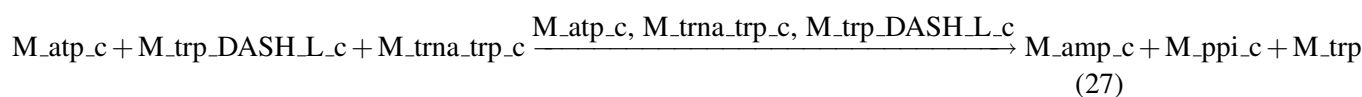
Id	Name	SBO	Value	Unit	Constant
kcat	kcat		0.043		<input checked="" type="checkbox"/>

### 6.14 Reaction R03664

This is an irreversible reaction of three reactants forming three products influenced by three modifiers.

**Name** WARS

#### Reaction equation



#### Reactants

Table 57: Properties of each reactant.

Id	Name	SBO
M_atp_c	M_ATP	
M_trp_DASH_L_c	M_Trp	
M_trna_trp_c	M_tRNA	

#### Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
M_atp_c	M_ATP	
M_trna_trp_c	M_tRNA	
M_trp_DASH_L_c	M_Trp	

#### Products

Table 59: Properties of each product.

Id	Name	SBO
M_amp_c	M_AMP	

Id	Name	SBO
M_ppi_c	M_PPi	
M_trp_L_trna_c	M_Trp_tRNA	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{14} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{kcat} \cdot E\_T \cdot [M\_trp\_DASH\_L\_c] \cdot [M\_trna\_trp\_c] \cdot [M\_atp\_c] \cdot \text{scaling}}{K_a \cdot K_b + K_b \cdot [M\_trp\_DASH\_L\_c] + K_a \cdot [M\_trna\_trp\_c] + [M\_trp\_DASH\_L\_c] \cdot [M\_trna\_trp\_c]} \quad (28)$$

Table 60: Properties of each parameter.

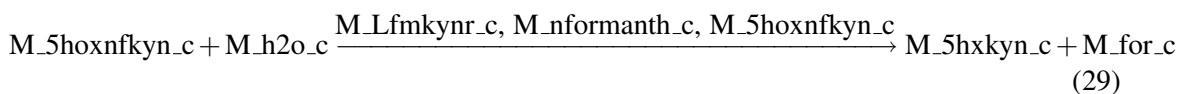
Id	Name	SBO	Value	Unit	Constant
E_T	E_T		15961.500		✓
Ka	Ka		0.007		✓
Kb	Kb		0.001		✓
kcat	kcat		1.100		✓

## 6.15 Reaction R04911

This is an irreversible reaction of two reactants forming two products influenced by three modifiers.

**Name** AFMID\_5HFKyn

## Reaction equation



## Reactants

Table 61: Properties of each reactant.

Id	Name	SBO
M_5hoxnfkyn_c	M_5HFKyn	
M_h2o_c	M_H2O	

## Modifiers

Table 62: Properties of each modifier.

Id	Name	SBO
M_Lfmkynr_c	M_FKyn	
M_nformanth_c	M_FAA	
M_5hoxnfkyn_c	M_5HFKyn	

## Products

Table 63: Properties of each product.

Id	Name	SBO
M_5hxxkyn_c	M_5HKyn	
M_for_c	M_Formate	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{15} = \text{vol}(\text{Cytosol}) \quad (30)$$

$$\frac{\text{AFMID\_E\_T} \cdot \text{kcat\_A}}{\text{AFMID\_Km\_5hoxnfky} \cdot \text{AFMID\_Km\_Lfmkynr} \cdot \text{AFMID\_Km\_nformanth} + \text{AFMID\_Km\_Lfmkynr} \cdot \text{AFMID\_Km\_5hxxkyn} + \text{AFMID\_Km\_for}}$$

Table 64: Properties of each parameter.

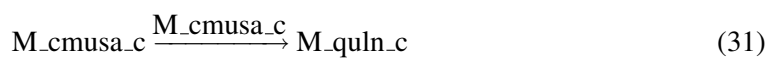
Id	Name	SBO	Value	Unit	Constant
kcat_A	kcat_A		100.0		<input checked="" type="checkbox"/>

### 6.16 Reaction `quin_form`

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

**Name** Quinolic Acid formation (spontaneous)

### Reaction equation





## Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
M_cmusa_c	M_Acms	

## Modifier

Table 66: Properties of each modifier.

Id	Name	SBO
M_cmusa_c	M_Acms	

## Product

Table 67: Properties of each product.

Id	Name	SBO
M_quln_c	M_Quin	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{16} = \text{vol}(\text{Cytosol}) \cdot k1 \cdot [\text{M\_cmusa\_c}] \quad (32)$$

Table 68: Properties of each parameter.

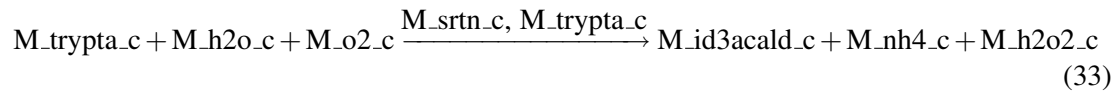
Id	Name	SBO	Value	Unit	Constant
k1	k1		$2.5 \cdot 10^{-4}$		✓

### 6.17 Reaction R02173\_Maoa

This is an irreversible reaction of three reactants forming three products influenced by two modifiers.

**Name** MAOA\_Trypta

## Reaction equation



## Reactants

Table 69: Properties of each reactant.

Id	Name	SBO
M_trypta_c	M_Trypta	
M_h2o_c	M_H2O	
M_o2_c	M_O2	

## Modifiers

Table 70: Properties of each modifier.

Id	Name	SBO
M_srt_n_c	M_Serotonin	
M_trypta_c	M_Trypta	

## Products

Table 71: Properties of each product.

Id	Name	SBO
M_id3acald_c	M_IndolAc	
M_nh4_c	M_NH4	
M_h2o2_c	M_H2O2	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{17} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{MAOA\_E\_T} \cdot \text{kcat\_B} \cdot \text{scaling} \cdot [M\_trypta\_c] \cdot \text{MAO\_Km\_srt}}{\text{MAO\_Km\_trypta} \cdot \text{MAO\_Km\_srt} + \text{MAO\_Km\_trypta} \cdot [M\_srt\_c] + \text{MAO\_Km\_srt} \cdot [M\_trypta\_c]} \quad (34)$$

Table 72: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat_B	kcat_B		3.5		<input checked="" type="checkbox"/>

### 6.18 Reaction R02670

This is an irreversible reaction of two reactants forming four products influenced by two modifiers.

**Name** Cinnavalinate formation

#### Reaction equation



#### Reactants

Table 73: Properties of each reactant.

Id	Name	SBO
M_3hanthrn_c	M_3HAA	
M_o2_c	M_O2	

#### Modifiers

Table 74: Properties of each modifier.

Id	Name	SBO
M_3hanthrn_c	M_3HAA	
M_o2_c	M_O2	

#### Products

Table 75: Properties of each product.

Id	Name	SBO
M_Cinnavalininate_c	M_Cin	
M_o2s_c	M_O2s	
M_h2o2_c	M_H2O2	

Id	Name	SBO
M_h_c	M_H	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{18} = \text{vol}(\text{Cytosol}) \cdot k1 \cdot [\text{M\_3hanthrn\_c}]^{e1} \cdot [\text{M\_o2\_c}]^{e2} \quad (36)$$

Table 76: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
e1	e1		2.000		<input checked="" type="checkbox"/>
e2	e2		4.000		<input checked="" type="checkbox"/>
k1	k1		$5.6667 \cdot 10^{-5}$		<input checked="" type="checkbox"/>

## 6.19 Reaction TRPtrans\_Slc7a5

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

**Name** Tryptophan\_Transport Slc7a5

## Reaction equation



## Reactant

Table 77: Properties of each reactant.

Id	Name	SBO
TRP_ex	Trp_ex	

## Modifiers

Table 78: Properties of each modifier.

Id	Name	SBO
M_Lkynr_ex	M_LKyn_ex	
M_Lkynr_c	M_L-Kyn	

Id	Name	SBO
M_trp_DASH.L_c	M.Trp	
TRP_ex	Trp_ex	

## Product

Table 79: Properties of each product.

Id	Name	SBO
M_trp_DASH.L_c	M.Trp	

## Kinetic Law

**Derived unit** contains undeclared units

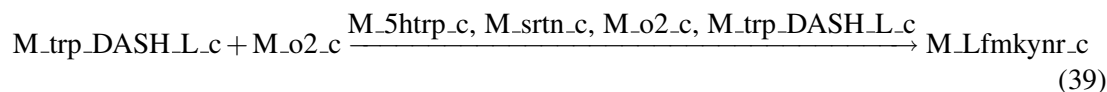
$$v_{19} = \text{vol}(\text{Cytosol}) \cdot \left( \frac{\text{Transporter\_E\_T\_Slc7a5} \cdot \text{Transporter\_kcat\_Trp} \cdot [\text{TRP\_ex}]}{\text{Transporter\_Km\_Trp\_Slc7a5}} - \frac{\text{Transporter\_E\_T\_Slc7a5} \cdot \text{Transporter\_kcat\_Trp} \cdot [\text{M\_trp\_DASH.L\_c}]}{\text{Transporter\_Km\_Trp\_Slc7a5}} \right) \cdot \frac{1}{1 + \frac{[\text{TRP\_ex}]}{\text{Transporter\_Km\_Trp\_Slc7a5}} + \frac{[\text{M\_Lkynr\_ex}]}{\text{Transporter\_Km\_Lkynr}} + \frac{[\text{M\_trp\_DASH.L\_c}]}{\text{Transporter\_Km\_Trp\_Slc7a5}} + \frac{[\text{M\_Lkynr\_c}]}{\text{Transporter\_Km\_Lkynr}}} \quad (38)$$

## 6.20 Reaction R00678\_Indo

This is an irreversible reaction of two reactants forming one product influenced by four modifiers.

**Name** IDO

## Reaction equation



## Reactants

Table 80: Properties of each reactant.

Id	Name	SBO
M_trp_DASH.L_c	M.Trp	
M_o2_c	M.O2	

## Modifiers

Table 81: Properties of each modifier.

Id	Name	SBO
M_5htrp_c	M_5HTrp	
M_srtm_c	M_Serotonin	
M_o2_c	M_O2	
M_trp_DASH_L_c	M_Trp	

## Product

Table 82: Properties of each product.

Id	Name	SBO
M_Lfmkynr_c	M_FKyn	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{20} = \text{vol}(\text{Cytosol}) \quad (40)$$

$$\frac{1}{\text{IDO\_Km\_trp\_DASH\_L} \cdot \text{IDO\_Km\_O2} \cdot \text{IDO\_Km\_5htrp} \cdot \text{IDO\_Km\_srtm} + [\text{M\_trp\_DASH\_L\_c}] \cdot \text{IDO\_Km\_O2} \cdot \text{IDO\_Km\_5htrp}}$$

Table 83: Properties of each parameter.

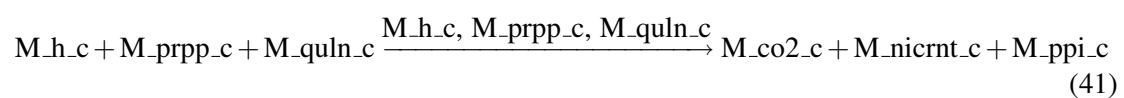
Id	Name	SBO	Value	Unit	Constant
kcat	kcat		1.65		<input checked="" type="checkbox"/>

## 6.21 Reaction R03348

This is an irreversible reaction of three reactants forming three products influenced by three modifiers.

**Name** QPRT

## Reaction equation



## Reactants

Table 84: Properties of each reactant.

Id	Name	SBO
M_h_c	M_H	
M_prpp_c	M_PRPP	
M_quln_c	M_Quin	

## Modifiers

Table 85: Properties of each modifier.

Id	Name	SBO
M_h_c	M_H	
M_prpp_c	M_PRPP	
M_quln_c	M_Quin	

## Products

Table 86: Properties of each product.

Id	Name	SBO
M_co2_c	M_CO2	
M_nicrnt_c	M_NaMN	
M_ppi_c	M_PPi	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{21} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{kcat} \cdot E_T \cdot [M_{\text{quln\_c}}] \cdot [M_{\text{prpp\_c}}] \cdot [M_{\text{h\_c}}] \cdot \text{scaling}}{K_a \cdot K_b + K_b \cdot [M_{\text{quln\_c}}] + K_a \cdot [M_{\text{prpp\_c}}] + [M_{\text{quln\_c}}] \cdot [M_{\text{prpp\_c}}]} \quad (42)$$

Table 87: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
E_T	E_T		138709.000		✓
Ka	Ka		0.022		✓
Kb	Kb		0.023		✓
kcat	kcat		0.255		✓

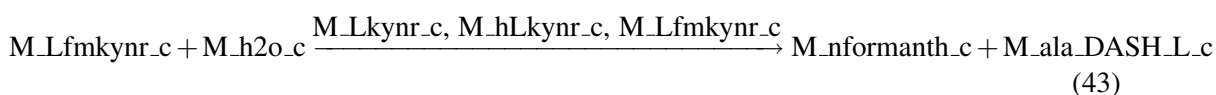


## 6.22 Reaction R03936

This is an irreversible reaction of two reactants forming two products influenced by three modifiers.

**Name** KYNU\_FKyn

### Reaction equation



### Reactants

Table 88: Properties of each reactant.

Id	Name	SBO
M_Lfmkynr_c	M_FKyn	
M_h2o_c	M_H2O	

### Modifiers

Table 89: Properties of each modifier.

Id	Name	SBO
M_Lkynr_c	M_L-Kyn	
M_hLkynr_c	M_3HKyn	
M_Lfmkynr_c	M_FKyn	

### Products

Table 90: Properties of each product.

Id	Name	SBO
M_nformanth_c	M_FAA	
M_ala_DASH_L_c	M_L_ALA	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{22} = \text{vol}(\text{Cytosol}) \quad (44)$$

$$\frac{\text{KYNu\_E\_T} \cdot \text{kcAt\_A} \cdot \text{scaling} \cdot [\text{M}]}{\text{KYNu\_Km\_Lfmkynr} \cdot \text{KYNu\_Km\_Lkynr} \cdot \text{KYNu\_Km\_hLkynr} + \text{KYNu\_Km\_Lkynr} \cdot \text{KYNu\_Km\_hLkynr} \cdot [\text{M}]}$$

Table 91: Properties of each parameter.

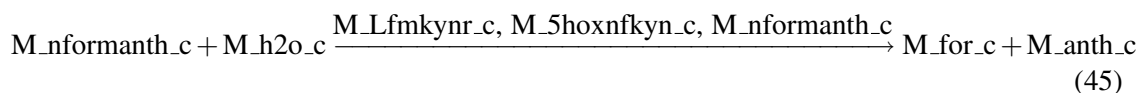
Id	Name	SBO	Value	Unit	Constant
kcat_A	kcat_A		0.013		<input checked="" type="checkbox"/>

### 6.23 Reaction R00988

This is an irreversible reaction of two reactants forming two products influenced by three modifiers.

**Name** AFMID\_FAA

## Reaction equation



## Reactants

Table 92: Properties of each reactant.

Id	Name	SBO
M_nformanth_c	M.FAA	
M_h2o_c	M.H2O	

## Modifiers

Table 93: Properties of each modifier.

Id	Name	SBO
M_Lfmkynr_c	M_FKyn	
M_5hoxnfkyn_c	M_5HFKyn	
M_nformanth_c	M_FAA	

## Products

Table 94: Properties of each product.

Id	Name	SBO
M_for_c	M_Formate	
M_anth_c	M_AA	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{23} = \text{vol}(\text{Cytosol}) \quad (46)$$

$$\frac{\text{AFMID\_E\_T} \cdot \text{kcat\_A}}{\text{AFMID\_Km\_nformanth} \cdot \text{AFMID\_Km\_Lfmkynr} \cdot \text{AFMID\_Km\_5hoxnfky} + \text{AFMID\_Km\_Lfmkynr} \cdot \text{AFMID\_Km\_5hoxnfky} \cdot \text{AFMID\_Km\_Lfmkynr}}$$

Table 95: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat_A	kcat_A		13.57		<input checked="" type="checkbox"/>

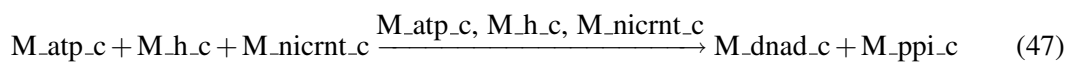
## 6.24 Reaction R03005

This is an irreversible reaction of three reactants forming two products influenced by three modifiers.

**Name** NMNAT1

**Notes** Km and kcat values taken from 17402747

## Reaction equation



## Reactants

Table 96: Properties of each reactant.

Id	Name	SBO
M_atp_c	M_ATP	
M_h_c	M_H	
M_nicrnt_c	M_NaMN	

## Modifiers

Table 97: Properties of each modifier.

Id	Name	SBO
M_atp_c	M_ATP	
M_h_c	M_H	
M_nicrnt_c	M_NaMN	

## Products

Table 98: Properties of each product.

Id	Name	SBO
M_dnad_c	M_NAAD	
M_ppi_c	M_PPi	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{24} = \text{vol}(\text{Cytosol}) \cdot \frac{E\_T \cdot kcat \cdot [M\_nicrnt\_c] \cdot [M\_h\_c] \cdot [M\_atp\_c] \cdot \text{scaling}}{K_m + [M\_nicrnt\_c]} \quad (48)$$

Table 99: Properties of each parameter.

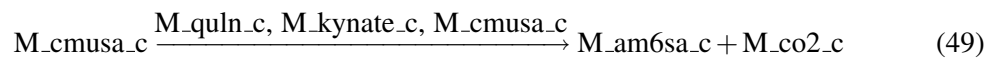
Id	Name	SBO	Value	Unit	Constant
E_T	E_T		4658.650		✓
Km	Km		0.068		✓
kcat	kcat		42.900		✓

### 6.25 Reaction R04323

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

**Name** ACMSD

#### Reaction equation



## Reactant

Table 100: Properties of each reactant.

Id	Name	SBO
M_cmusa_c	M_Acms	

## Modifiers

Table 101: Properties of each modifier.

Id	Name	SBO
M_quln_c	M_Quin	
M_kynate_c	M_Kyna	
M_cmusa_c	M_Acms	

## Products

Table 102: Properties of each product.

Id	Name	SBO
M_am6sa_c	M_Am6sa	
M_co2_c	M_CO2	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{25} = \text{vol}(\text{Cytosol}) \cdot \frac{E\_T \cdot kcat \cdot [M\_cmusa\_c] \cdot \text{scaling}}{K_m + [M\_cmusa\_c]} \quad (50)$$

Table 103: Properties of each parameter.

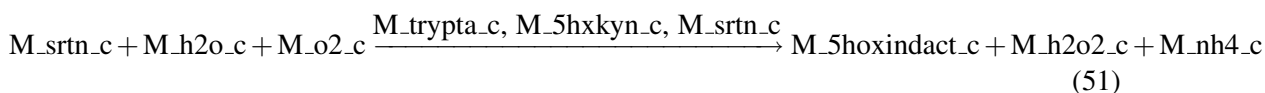
Id	Name	SBO	Value	Unit	Constant
E_T	E_T		48858.200		✓
Km	Km		0.007		✓
kcat	kcat		1.000		✓

## 6.26 Reaction R02908\_Maoa

This is an irreversible reaction of three reactants forming three products influenced by three modifiers.

**Name** MAOA\_Serotonin

### Reaction equation



### Reactants

Table 104: Properties of each reactant.

Id	Name	SBO
M_srtn_c	M.Serotonin	
M_h2o_c	M.H2O	
M_o2_c	M.O2	

### Modifiers

Table 105: Properties of each modifier.

Id	Name	SBO
M_trypta_c	M.Trypta	
M_5hxykn_c	M.5HKyn	
M_srtn_c	M.Serotonin	

### Products

Table 106: Properties of each product.

Id	Name	SBO
M_5hoxindact_c	M.5HAc	
M_h2o2_c	M.H2O2	
M_nh4_c	M.NH4	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{26} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{MAOA\_E\_T} \cdot \text{kcat\_B} \cdot \text{scaling} \cdot [\text{M\_srtn\_c}] \cdot \text{MAO\_Km\_trypta}}{\text{MAO\_Km\_srtn} \cdot \text{MAO\_Km\_trypta} + \text{MAO\_Km\_srtn} \cdot [\text{M\_trypta\_c}] + \text{MAO\_Km\_trypta} \cdot [\text{M\_srtn\_c}]} \quad (52)$$

Table 107: Properties of each parameter.

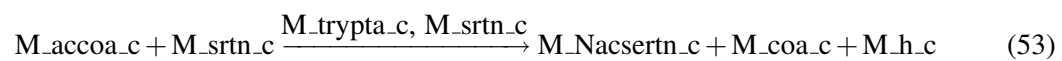
Id	Name	SBO	Value	Unit	Constant
kcat_B	kcat_B		18.6		<input checked="" type="checkbox"/>

## 6.27 Reaction R02911

This is an irreversible reaction of two reactants forming three products influenced by two modifiers.

**Name** AANAT\_Serotonin

### Reaction equation



### Reactants

Table 108: Properties of each reactant.

Id	Name	SBO
M_accoa_c	M_AcetylCoA	
M_srtn_c	M_Serotonin	

### Modifiers

Table 109: Properties of each modifier.

Id	Name	SBO
M_trypta_c	M_Trypta	
M_srtn_c	M_Serotonin	

### Products

Table 110: Properties of each product.

Id	Name	SBO
M_Nacsertn_c	M_NAcSet	
M_coa_c	M_CoA	
M_h_c	M_H	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{27} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{AANAT\_E\_T} \cdot \text{kcat\_B} \cdot \text{scaling} \cdot [\text{M\_srt\_c}] \cdot \text{AANAT\_Km\_trypta}}{\text{AANAT\_Km\_Srt\_n} \cdot \text{AANAT\_Km\_trypta} + \text{AANAT\_Km\_Srt\_n} \cdot [\text{M\_trypta\_c}] + \text{AANAT\_Km\_trypta} \cdot [\text{M\_srt\_c}]} \quad (54)$$

Table 111: Properties of each parameter.

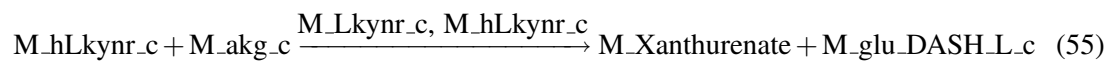
Id	Name	SBO	Value	Unit	Constant
kcat_B	kcat_B		25.9		<input checked="" type="checkbox"/>

## 6.28 Reaction R04171\_Kat1

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

**Name** KAT1\_3HKyn

## Reaction equation



## Reactants

Table 112: Properties of each reactant.

Id	Name	SBO
M_hLkynr_c	M_3HKyn	
M_akg_c	M_Ketoglutarate	

## Modifiers



Table 113: Properties of each modifier.

Id	Name	SBO
M_Lkynr_c	M_L-Kyn	
M_hLkynr_c	M_3HKyn	

## Products

Table 114: Properties of each product.

Id	Name	SBO
M_Xanthurenate	M_Xanth	
M_glu_DASH_L_c	M_LGlu	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{28} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{AADAT\_E\_T\_kat1} \cdot \text{AADAT\_kcat\_hLkynr} \cdot \text{scaling} \cdot [\text{M\_hLkynr\_c}] \cdot \text{AADAT\_Km\_Lkynr}}{\text{AADAT\_Km\_hLkynr} \cdot \text{AADAT\_Km\_Lkynr} + \text{AADAT\_Km\_hLkynr} \cdot [\text{M\_Lkynr\_c}] + \text{AADAT\_Km\_Lkynr} \cdot [\text{M\_hLkynr\_c}]} \quad (56)$$

### 6.29 Reaction R02909

This is an irreversible reaction of two reactants forming one product influenced by four modifiers.

**Name** IDO\_Serotonin

### Reaction equation



## Reactants

Table 115: Properties of each reactant.

Id	Name	SBO
M_srtn_c	M_Serotonin	
M_o2_c	M_O2	

## Modifiers

Table 116: Properties of each modifier.

Id	Name	SBO
M_5htrp_c	M_5HTrp	
M_trp_DASH_L_c	M_Trp	
M_o2_c	M_O2	
M_srtm_c	M_Serotonin	

## Product

Table 117: Properties of each product.

Id	Name	SBO
M_f5hoxkyn_c	M_F5HKyn	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{29} = \text{vol}(\text{Cytosol}) \quad (58)$$

$$\frac{1}{\text{IDO\_Km\_srtm} \cdot \text{IDO\_Km\_O2} \cdot \text{IDO\_Km\_5htrp} \cdot \text{IDO\_Km\_trp\_DASH\_L} + [\text{M\_srtm\_c}] \cdot \text{IDO\_Km\_O2} \cdot \text{IDO\_Km\_5htrp}}$$

Table 118: Properties of each parameter.

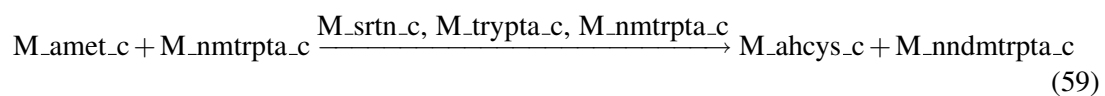
Id	Name	SBO	Value	Unit	Constant
kcat	kcat		0.002		<input checked="" type="checkbox"/>

### 6.30 Reaction R02174\_metTrypta

This is an irreversible reaction of two reactants forming two products influenced by three modifiers.

**Name** INMT\_MTrypta

#### Reaction equation



## Reactants

Table 119: Properties of each reactant.

Id	Name	SBO
M_amet_c	M_AMet	
M_nmtrpta_c	M_MTrypta	

## Modifiers

Table 120: Properties of each modifier.

Id	Name	SBO
M_srtm_c	M_Serotonin	
M_trypta_c	M_Trypta	
M_nmtrpta_c	M_MTrypta	

## Products

Table 121: Properties of each product.

Id	Name	SBO
M_ahcys_c	M_AHCys	
M_nndmtrpta_c	M_MMTrypta	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{30} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{IMNT\_E\_T} \cdot \text{kcat\_A} \cdot \text{scaling} \cdot [\text{M\_nmtrpta\_c}]}{\text{IMNT\_Km\_nmtrpta} \cdot \text{IMNT\_Km\_srtm} \cdot \text{IMNT\_Km\_trypta} + \text{IMNT\_Km\_srtm} \cdot \text{IMNT\_Km\_trypta} \cdot [\text{M\_nmtrpta\_c}]} \quad (60)$$

Table 122: Properties of each parameter.

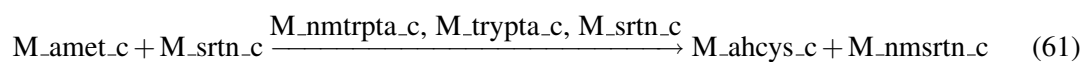
Id	Name	SBO	Value	Unit	Constant
kcat_A	kcat_A		0.176		<input checked="" type="checkbox"/>

### 6.31 Reaction R02910

This is an irreversible reaction of two reactants forming two products influenced by three modifiers.

**Name** INMT\_Serotonin

#### Reaction equation



#### Reactants

Table 123: Properties of each reactant.

Id	Name	SBO
M_amet_c	M_AMet	
M_srtn_c	M_Serotonin	

#### Modifiers

Table 124: Properties of each modifier.

Id	Name	SBO
M_nmtrpta_c	M_MTrypta	
M_trypta_c	M_Trypta	
M_srtn_c	M_Serotonin	

#### Products

Table 125: Properties of each product.

Id	Name	SBO
M_ahcys_c	M_AHCys	
M_nmsrtn_c	M_NMSer	

#### Kinetic Law

**Derived unit** contains undeclared units



Table 129: Properties of each product.

Id	Name	SBO
M_Xanthurenate	M_Xanth	
M_glu_DASH_L_c	M_LGlu	

## Kinetic Law

**Derived unit** contains undeclared units

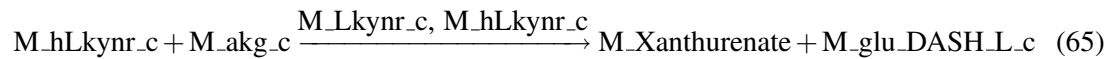
$$v_{32} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{AADAT\_E\_T\_kat2} \cdot \text{AADAT\_kcat\_hLkynr} \cdot \text{scaling} \cdot [\text{M\_hLkynr\_c}] \cdot \text{AADAT\_Km\_Lkynr}}{\text{AADAT\_Km\_hLkynr} \cdot \text{AADAT\_Km\_Lkynr} + \text{AADAT\_Km\_hLkynr} \cdot [\text{M\_Lkynr\_c}] + \text{AADAT\_Km\_Lkynr} \cdot [\text{M\_hLkynr\_c}]} \quad (64)$$

### 6.33 Reaction R01956\_Kat3

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

**Name** KAT3\_3HKyn

## Reaction equation



## Reactants

Table 130: Properties of each reactant.

Id	Name	SBO
M_hLkynr_c	M_3HKyn	
M_akg_c	M_Ketoglutarate	

## Modifiers

Table 131: Properties of each modifier.

Id	Name	SBO
M_Lkynr_c	M_L-Kyn	
M_hLkynr_c	M_3HKyn	

## Products

Table 132: Properties of each product.

Id	Name	SBO
M_Xanthurenate	M_Xanth	
M_glu_DASH_L_c	M_LGlu	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{33} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{AADAT\_E\_T\_kat3} \cdot \text{AADAT\_kcat\_hLkynr} \cdot \text{scaling} \cdot [\text{M\_hLkynr\_c}] \cdot \text{AADAT\_Km\_Lkynr}}{\text{AADAT\_Km\_hLkynr} \cdot \text{AADAT\_Km\_Lkynr} + \text{AADAT\_Km\_hLkynr} \cdot [\text{M\_Lkynr\_c}] + \text{AADAT\_Km\_Lkynr} \cdot [\text{M\_hLkynr\_c}]} \quad (66)$$

### 6.34 Reaction R04171\_Kat2

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

**Name** KAT2\_L-Kyn

## Reaction equation



## Reactants

Table 133: Properties of each reactant.

Id	Name	SBO
M_Lkynr_c	M_L-Kyn	
M_akg_c	M_Ketoglutarate	

## Modifiers

Table 134: Properties of each modifier.

Id	Name	SBO
M_hLkynr_c	M_3HKyn	
M_Lkynr_c	M_L-Kyn	

## Products

Table 135: Properties of each product.

Id	Name	SBO
M_kynate_c	M_Kyna	
M_glu_DASH_L_c	M_LGlu	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{34} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{AADAT\_E\_T\_kat2} \cdot \text{AADAT\_kcat\_Lkynr} \cdot \text{scaling} \cdot [\text{M\_Lkynr\_c}] \cdot \text{AADAT\_Km\_hLkynr}}{\text{AADAT\_Km\_Lkynr} \cdot \text{AADAT\_Km\_hLkynr} + \text{AADAT\_Km\_Lkynr} \cdot [\text{M\_hLkynr\_c}] + \text{AADAT\_Km\_hLkynr} \cdot [\text{M\_Lkynr\_c}]} \quad (68)$$

### 6.35 Reaction R04171\_Kat3

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

**Name** KAT3\_L-Kyn

## Reaction equation



## Reactants

Table 136: Properties of each reactant.

Id	Name	SBO
M_Lkynr_c	M_L-Kyn	
M_akg_c	M_Ketoglutarate	

## Modifiers

Table 137: Properties of each modifier.

Id	Name	SBO
M_hLkynr_c	M_3HKyn	
M_Lkynr_c	M_L-Kyn	



## Products

Table 138: Properties of each product.

Id	Name	SBO
M_kynate_c	M_Kyna	
M_glu_DASH_L_c	M_LGlu	

## Kinetic Law

**Derived unit** contains undeclared units

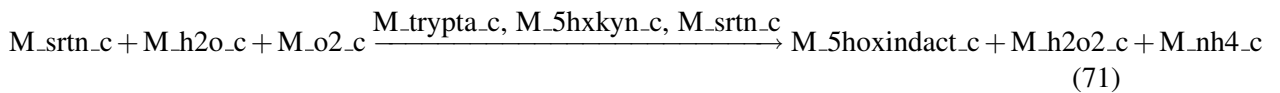
$$v_{35} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{AADAT\_E\_T\_kat3} \cdot \text{AADAT\_kcat\_Lkynr} \cdot \text{scaling} \cdot [\text{M\_Lkynr\_c}] \cdot \text{AADAT\_Km\_hLkynr}}{\text{AADAT\_Km\_Lkynr} \cdot \text{AADAT\_Km\_hLkynr} + \text{AADAT\_Km\_Lkynr} \cdot [\text{M\_hLkynr\_c}] + \text{AADAT\_Km\_hLkynr} \cdot [\text{M\_Lkynr\_c}]} \quad (70)$$

### 6.36 Reaction R02908\_Maob

This is an irreversible reaction of three reactants forming three products influenced by three modifiers.

**Name** MAOB\_Serotonin

## Reaction equation



## Reactants

Table 139: Properties of each reactant.

Id	Name	SBO
M_srtn_c	M_Serotonin	
M_h2o_c	M_H2O	
M_o2_c	M_O2	

## Modifiers

Table 140: Properties of each modifier.

Id	Name	SBO
M_trypta_c	M_Trypta	
M_5hxykn_c	M_5HKyn	
M_srtm_c	M_Serotonin	

## Products

Table 141: Properties of each product.

Id	Name	SBO
M_5hoxindact_c	M_5HAc	
M_h2o2_c	M_H2O2	
M_nh4_c	M_NH4	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{36} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{MAOB\_E.T} \cdot \text{kcat\_B} \cdot \text{scaling} \cdot [\text{M\_srtm\_c}] \cdot \text{MAO\_Km\_trypta}}{\text{MAO\_Km\_srtm} \cdot \text{MAO\_Km\_trypta} + \text{MAO\_Km\_srtm} \cdot [\text{M\_trypta\_c}] + \text{MAO\_Km\_trypta} \cdot [\text{M\_srtm\_c}]} \quad (72)$$

Table 142: Properties of each parameter.

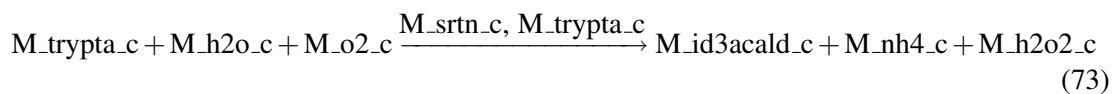
Id	Name	SBO	Value	Unit	Constant
kcat_B	kcat_B		18.6		<input checked="" type="checkbox"/>

### 6.37 Reaction R02173\_Maob

This is an irreversible reaction of three reactants forming three products influenced by two modifiers.

**Name** MAOB\_Trypta

#### Reaction equation



## Reactants

Table 143: Properties of each reactant.

Id	Name	SBO
M_trypta_c	M_Trypta	
M_h2o_c	M_H2O	
M_o2_c	M_O2	

## Modifiers

Table 144: Properties of each modifier.

Id	Name	SBO
M_srtm_c	M_Serotonin	
M_trypta_c	M_Trypta	

## Products

Table 145: Properties of each product.

Id	Name	SBO
M_id3acald_c	M_IndolAc	
M_nh4_c	M_NH4	
M_h2o2_c	M_H2O2	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{37} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{MAOB\_E\_T} \cdot \text{kcat\_B} \cdot \text{scaling} \cdot [\text{M\_trypta\_c}] \cdot \text{MAO\_Km\_srtm}}{\text{MAO\_Km\_trypta} \cdot \text{MAO\_Km\_srtm} + \text{MAO\_Km\_trypta} \cdot [\text{M\_srtm\_c}] + \text{MAO\_Km\_srtm} \cdot [\text{M\_trypta\_c}]} \quad (74)$$

Table 146: Properties of each parameter.

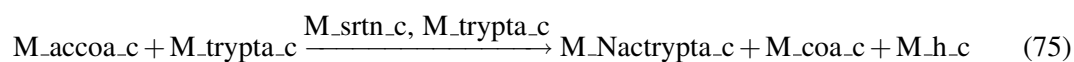
Id	Name	SBO	Value	Unit	Constant
kcat_B	kcat_B		3.5		✓

### 6.38 Reaction AANAT\_Trypta

This is an irreversible reaction of two reactants forming three products influenced by two modifiers.

**Name** AANAT\_Trypta

#### Reaction equation



#### Reactants

Table 147: Properties of each reactant.

Id	Name	SBO
M_accoa_c	M_AcetylCoA	
M_trypta_c	M_Trypta	

#### Modifiers

Table 148: Properties of each modifier.

Id	Name	SBO
M_srtn_c	M_Serotonin	
M_trypta_c	M_Trypta	

#### Products

Table 149: Properties of each product.

Id	Name	SBO
M_Nactrypta_c	M_Nactrypta	
M_coa_c	M_CoA	
M_h_c	M_H	

#### Kinetic Law

**Derived unit** contains undeclared units

$$v_{38} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{AANAT\_E\_T} \cdot \text{kcat\_B} \cdot \text{scaling} \cdot [\text{M\_trypta\_c}] \cdot \text{AANAT\_Km\_Srtn}}{\text{AANAT\_Km\_trypta} \cdot \text{AANAT\_Km\_Srtn} + \text{AANAT\_Km\_trypta} \cdot [\text{M\_srtn\_c}] + \text{AANAT\_Km\_Srtn} \cdot [\text{M\_trypta\_c}]} \quad (76)$$

Table 150: Properties of each parameter.

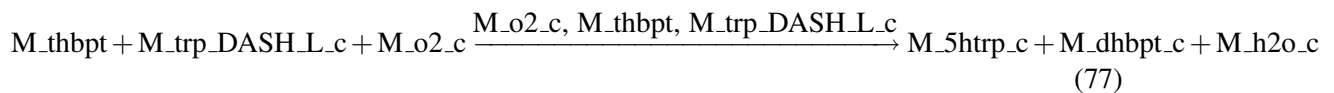
Id	Name	SBO	Value	Unit	Constant
kcat_B	kcat_B		25.9		<input checked="" type="checkbox"/>

### 6.39 Reaction R01814\_Tph2

This is an irreversible reaction of three reactants forming three products influenced by three modifiers.

**Name** TPH2

#### Reaction equation



#### Reactants

Table 151: Properties of each reactant.

Id	Name	SBO
M_thbpt	M_Thbpt	
M_trp_DASH_L_c	M_Trp	
M_o2_c	M_O2	

#### Modifiers

Table 152: Properties of each modifier.

Id	Name	SBO
M_o2_c	M_O2	
M_thbpt	M_Thbpt	
M_trp_DASH_L_c	M_Trp	

#### Products

Table 153: Properties of each product.

Id	Name	SBO
M_5htrp_c	M_5HTrp	
M_dhbpt_c	M_Dhbpt	
M_h2o_c	M_H2O	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{39} = \text{vol}(\text{Cytosol}) \cdot \frac{\text{kcat} \cdot E\_T \cdot [M\_trp\_DASH\_L\_c] \cdot [M\_o2\_c] \cdot [M\_thbpt] \cdot \text{scaling}}{K_a \cdot K_b + K_b \cdot [M\_trp\_DASH\_L\_c] + K_a \cdot [M\_o2\_c] + [M\_trp\_DASH\_L\_c] \cdot [M\_o2\_c]} \quad (78)$$

Table 154: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
E_T	E_T		235.128		✓
Ka	Ka		0.040		✓
Kb	Kb		0.273		✓
kcat	kcat		0.180		✓

### 6.40 Reaction TRPtrans\_Slc7a8

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

**Name** Tryptophan\_Transport Slc7a8

### Reaction equation



### Reactant

Table 155: Properties of each reactant.

Id	Name	SBO
TRP_ex	Trp_ex	

## Modifiers

Table 156: Properties of each modifier.

Id	Name	SBO
M_Lkynr_ex	M.LKyn_ex	
M_Lkynr_c	M.L-Kyn	
M_trp_DASH.L_c	M.Trp	
TRP_ex	Trp_ex	

## Product

Table 157: Properties of each product.

Id	Name	SBO
M_trp_DASH.L_c	M.Trp	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{40} = \text{vol}(\text{Cytosol}) \cdot \text{scaling} \cdot \left( \frac{\text{Transporter\_E\_T\_Slc7a8} \cdot \text{Transporter\_kcat\_Trp} \cdot [\text{TRP\_ex}]}{\text{Transporter\_Km\_Trp\_Slc7a8}} - \frac{\text{Transporter\_E\_T\_Slc7a8} \cdot \text{Transporter\_kcat\_Trp} \cdot [\text{M\_trp\_DASH.L\_c}]}{\text{Transporter\_Km\_Trp\_Slc7a8}} \right) \cdot \frac{1}{1 + \frac{[\text{TRP\_ex}]}{\text{Transporter\_Km\_Trp\_Slc7a8}} + \frac{[\text{M\_Lkynr\_ex}]}{\text{Transporter\_Km\_Lkynr}} + \frac{[\text{M\_trp\_DASH.L\_c}]}{\text{Transporter\_Km\_Trp\_Slc7a8}} + \frac{[\text{M\_Lkynr\_c}]}{\text{Transporter\_Km\_Lkynr}}} \quad (80)$$

### 6.41 Reaction Lkynr\_trans\_Slc7a5

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

**Name** Lkynr\_Transporter\_Slc7a5

### Reaction equation



## Reactant

Table 158: Properties of each reactant.

Id	Name	SBO
M_Lkynr_c	M.L-Kyn	

## Modifiers

Table 159: Properties of each modifier.

Id	Name	SBO
M_trp_DASH_L_c	M.Trp	
TRP_ex	Trp_ex	
M_Lkynr_c	M.L-Kyn	
M_Lkynr_ex	M.LKyn_ex	

## Product

Table 160: Properties of each product.

Id	Name	SBO
M_Lkynr_ex	M.LKyn_ex	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{41} = \text{vol}(\text{Cytosol}) \cdot \text{scaling} \cdot \left( \frac{\text{Transporter\_E\_T\_Slc7a5} \cdot \text{Transporter\_kcat\_Lkynr} \cdot [\text{M\_Lkynr\_c}]}{\text{Transporter\_Km\_Lkynr}} - \frac{\text{Transporter\_E\_T\_Slc7a5} \cdot \text{Transporter\_kcat\_Lkynr} \cdot [\text{M\_Lkynr\_ex}]}{\text{Transporter\_Km\_Lkynr}} \right) \cdot \frac{1}{1 + \frac{[\text{M\_Lkynr\_c}]}{\text{Transporter\_Km\_Lkynr}} + \frac{[\text{M\_trp\_DASH\_L\_c}]}{\text{Transporter\_Km\_Trp\_Slc7a5}} + \frac{[\text{M\_Lkynr\_ex}]}{\text{Transporter\_Km\_Lkynr}} + \frac{[\text{TRP\_ex}]}{\text{Transporter\_Km\_Trp\_Slc7a5}}} \quad (82)$$

### 6.42 Reaction Lkynr\_trans\_Slc7a8

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

**Name** Lkynr\_Transporter\_Slc7a8

### Reaction equation



## Reactant

Table 161: Properties of each reactant.

Id	Name	SBO
M_Lkynr_c	M.L-Kyn	



## Modifiers

Table 162: Properties of each modifier.

Id	Name	SBO
M_trp_DASH.L_c	M.Trp	
TRP_ex	Trp_ex	
M_Lkynr_c	M.L-Kyn	
M_Lkynr_ex	M.LKyn_ex	

## Product

Table 163: Properties of each product.

Id	Name	SBO
M_Lkynr_ex	M.LKyn_ex	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{42} = \text{vol}(\text{Cytosol}) \cdot \text{scaling} \cdot \left( \frac{\text{Transporter\_E\_T\_Slc7a8} \cdot \text{Transporter\_kcat\_Lkynr} \cdot [\text{M\_Lkynr\_c}]}{\text{Transporter\_Km\_Lkynr}} - \frac{\text{Transporter\_E\_T\_Slc7a8} \cdot \text{Transporter\_kcat\_Lkynr} \cdot [\text{M\_Lkynr\_ex}]}{\text{Transporter\_Km\_Lkynr}} \right) \quad (84)$$

$$\cdot \frac{1}{1 + \frac{[\text{M\_Lkynr\_c}]}{\text{Transporter\_Km\_Lkynr}} + \frac{[\text{M\_trp\_DASH.L\_c}]}{\text{Transporter\_Km\_Trp\_Slc7a8}} + \frac{[\text{M\_Lkynr\_ex}]}{\text{Transporter\_Km\_Lkynr}} + \frac{[\text{TRP\_ex}]}{\text{Transporter\_Km\_Trp\_Slc7a8}}}$$

## 7 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML substance per time. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or
- volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions` > 0 for certain species.

### 7.1 Species M\_3hanthrn\_c

**Name** M\_3HAA

**Initial concentration**  $3.29767682642125 \cdot 10^{-6} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [R02665](#), [R02670](#) and as a product in [R02668](#) and as a modifier in [R02665](#), [R02670](#)).

$$\frac{d}{dt} \text{M\_3hanthrn\_c} = v_{11} - v_{10} - 2 v_{18} \quad (85)$$

## 7.2 Species [M\\_5hoxnfkyn\\_c](#)

**Name** M\_5HFKyn

**Initial concentration**  $2.3285262897484 \cdot 10^{-10} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [R04911](#) and as a product in [R02702](#) and as a modifier in [R01959](#), [R04911](#), [R00988](#)).

$$\frac{d}{dt} \text{M\_5hoxnfkyn\_c} = v_{13} - v_{15} \quad (86)$$

## 7.3 Species [M\\_5htrp\\_c](#)

**Name** M\_5HTrp

**Initial concentration**  $9.86485434437397 \cdot 10^{-7} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in nine reactions (as a reactant in [R02701](#), [R02702](#) and as a product in [R01814\\_Tph1](#), [R01814\\_Tph2](#) and as a modifier in [R00685](#), [R02701](#), [R02702](#), [R00678\\_Indo](#), [R02909](#)).

$$\frac{d}{dt} \text{M\_5htrp\_c} = v_5 + v_{39} - v_{12} - v_{13} \quad (87)$$

## 7.4 Species [M\\_5hxxkyn\\_c](#)

**Name** M\_5HKyn

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

This species takes part in three reactions (as a product in [R04911](#) and as a modifier in [R02908\\_Maoa](#), [R02908\\_Maob](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{M\_5hxxkyn\_c} = 0 \quad (88)$$

## 7.5 Species `M_Lfmkynr_c`

**Name** `M_FKyn`

**Initial concentration**  $2.18400152663056 \cdot 10^{-5} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in ten reactions (as a reactant in [R01959](#), [R03936](#) and as a product in [R00678\\_Tdo](#), [R00678\\_Indo](#) and as a modifier in [R00987](#), [R01959](#), [R02668](#), [R04911](#), [R03936](#), [R00988](#)).

$$\frac{d}{dt} \text{M\_Lfmkynr\_c} = v_2 + v_{20} - v_7 - v_{22} \quad (89)$$

## 7.6 Species `M_Lkynr_c`

**Name** `M_L-Kyn`

**Initial concentration**  $0.00263243682881056 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in 22 reactions (as a reactant in [R00987](#), [R01956\\_Kat1](#), [R01960](#), [R04171-Kat2](#), [R04171\\_Kat3](#), [Lkynr\\_trans\\_Slc7a5](#), [Lkynr\\_trans\\_Slc7a8](#) and as a product in [R01959](#) and as a modifier in [R00987](#), [R01956\\_Kat1](#), [R01960](#), [R02668](#), [TRPtrans\\_Slc7a5](#), [R03936](#), [R04171\\_Kat1](#), [R01956\\_Kat2](#), [R01956\\_Kat3](#), [R04171\\_Kat2](#), [R04171\\_Kat3](#), [TRPtrans\\_Slc7a8](#), [Lkynr\\_trans\\_Slc7a5](#), [Lkynr\\_trans\\_Slc7a8](#)).

$$\frac{d}{dt} \text{M\_Lkynr\_c} = v_7 - v_4 - v_6 - v_8 - v_{34} - v_{35} - v_{41} - v_{42} \quad (90)$$

## 7.7 Species `M_ahcys_c`

**Name** `M_AHCys`

**Initial concentration**  $1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a product in [R02174](#), [R02174\\_metTrypta](#), [R02910](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{M\_ahcys\_c} = 0 \quad (91)$$

## 7.8 Species `M_akg_c`

**Name** `M_Ketoglutarate`

**Initial concentration**  $0.9999999518 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in [R01956\\_Kat1](#), [R04171\\_Kat1](#), [R01956-Kat2](#), [R01956\\_Kat3](#), [R04171\\_Kat2](#), [R04171\\_Kat3](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{M\_akg\_c} = 0 \quad (92)$$

## 7.9 Species `M_ala_DASH_L_c`

**Name** `M_L_ALA`

**Initial concentration**  $1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a product in [R00987](#), [R02668](#), [R03936](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_ala\_DASH\_L\_c = 0 \quad (93)$$

## 7.10 Species `M_amet_c`

**Name** `M_AMet`

**Initial concentration**  $0.9999999518 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [R02174](#), [R02174\\_metTrypta](#), [R02910](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_amet\_c = 0 \quad (94)$$

## 7.11 Species `M_anth_c`

**Name** `M_AA`

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

This species takes part in three reactions (as a product in [R00987](#), [R00988](#) and as a modifier in [R02665](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_anth\_c = 0 \quad (95)$$

## 7.12 Species `M_cmusa_c`

**Name** `M_Acms`

**Initial concentration**  $1.12181722190904 \cdot 10^{-5} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [quin\\_form](#), [R04323](#) and as a product in [R02665](#) and as a modifier in [quin\\_form](#), [R04323](#)).

$$\frac{d}{dt}M\_cmusa\_c = v_{10} - v_{16} - v_{25} \quad (96)$$

### 7.13 Species [M\\_dhbpt\\_c](#)

**Name** M\_Dhbpt

**Initial concentration** 1 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a product in [R01814\\_Tph1](#), [R01814\\_Tph2](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_dhbpt\_c = 0 \quad (97)$$

### 7.14 Species [M\\_for\\_c](#)

**Name** M\_Formate

**Initial concentration** 0 mmol · l<sup>-1</sup>

This species takes part in three reactions (as a product in [R01959](#), [R04911](#), [R00988](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_for\_c = 0 \quad (98)$$

### 7.15 Species [M\\_glu\\_DASH\\_L\\_c](#)

**Name** M\_LGlu

**Initial concentration** 0 mmol · l<sup>-1</sup>

This species takes part in six reactions (as a product in [R01956\\_Kat1](#), [R04171\\_Kat1](#), [R01956\\_Kat2](#), [R01956\\_Kat3](#), [R04171\\_Kat2](#), [R04171\\_Kat3](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_glu\_DASH\_L\_c = 0 \quad (99)$$

### 7.16 Species [M\\_hLkynr\\_c](#)

**Name** M\_3HKyn

**Initial concentration** 1.1966020248522 · 10<sup>-5</sup> mmol · l<sup>-1</sup>

This species takes part in 14 reactions (as a reactant in [R02668](#), [R04171\\_Kat1](#), [R01956\\_Kat2](#), [R01956\\_Kat3](#) and as a product in [R01960](#) and as a modifier in [R00987](#), [R01956\\_Kat1](#), [R02668](#), [R03936](#), [R04171\\_Kat1](#), [R01956\\_Kat2](#), [R01956\\_Kat3](#), [R04171\\_Kat2](#), [R04171\\_Kat3](#)).

$$\frac{d}{dt}M\_hLkynr\_c = v_8 - v_{11} - v_{28} - v_{32} - v_{33} \quad (100)$$

### 7.17 Species [M\\_id3acald\\_c](#)

**Name** M\_IndolAc

**Initial concentration** 0 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a product in [R02173\\_Maoa](#), [R02173\\_Maob](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{id3acald\_c} = 0 \quad (101)$$

### 7.18 Species [M\\_indpyr\\_c](#)

**Name** M\_IndolP

**Initial concentration** 0 mmol · l<sup>-1</sup>

This species takes part in one reaction (as a product in [R00677](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{indpyr\_c} = 0 \quad (102)$$

### 7.19 Species [M\\_nmtrpta\\_c](#)

**Name** M\_MTrypta

**Initial concentration** 2.5994745417821 · 10<sup>-9</sup> mmol · l<sup>-1</sup>

This species takes part in five reactions (as a reactant in [R02174\\_metTrypta](#) and as a product in [R02174](#) and as a modifier in [R02174](#), [R02174\\_metTrypta](#), [R02910](#)).

$$\frac{d}{dt}M_{nmtrpta\_c} = v_9 - v_{30} \quad (103)$$

### 7.20 Species [M\\_quln\\_c](#)

**Name** M\_Quin

**Initial concentration** 1.78449610733141 · 10<sup>-15</sup> mmol · l<sup>-1</sup>

This species takes part in five reactions (as a reactant in [R03348](#) and as a product in [quin\\_form](#) and as a modifier in [R02665](#), [R03348](#), [R04323](#)).

$$\frac{d}{dt}M_{quln\_c} = v_{16} - v_{21} \quad (104)$$

## 7.21 Species `M_srtnc`

**Name** `M_Serotonin`

**Initial concentration**  $7.76306594979262 \cdot 10^{-8} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in 18 reactions (as a reactant in [R02908\\_Maoa](#), [R02911](#), [R02909](#), [R02910](#), [R02908\\_Maob](#) and as a product in [R02701](#) and as a modifier in [R02174](#), [R02702](#), [R02173\\_Maoa](#), [R00678\\_Indo](#), [R02908\\_Maoa](#), [R02911](#), [R02909](#), [R02174\\_metTrypta](#), [R02910](#), [R02908\\_Maob](#), [R02173\\_Maob](#), [AANAT\\_Trypta](#)).

$$\frac{d}{dt}M_{\text{srtnc}} = v_{12} - v_{26} - v_{27} - v_{29} - v_{31} - v_{36} \quad (105)$$

## 7.22 Species `M_thbpt`

**Name** `M_Thbpt`

**Initial concentration**  $1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in [R01814\\_Tph1](#), [R01814\\_Tph2](#) and as a modifier in [R01814\\_Tph1](#), [R01814\\_Tph2](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{\text{thbpt}} = 0 \quad (106)$$

## 7.23 Species `M_trna_trp_c`

**Name** `M_tRNA`

**Initial concentration**  $10^{-5} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [R03664](#) and as a modifier in [R03664](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{\text{trna\_trp\_c}} = 0 \quad (107)$$

## 7.24 Species `M_trp_DASH_L_c`

**Name** `M_Trp`

**Initial concentration**  $1.20064386474403 \cdot 10^{-4} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in 23 reactions (as a reactant in [R00677](#), [R00678\\_Tdo](#), [R00685](#), [R01814\\_Tph1](#), [R03664](#), [R00678\\_Indo](#), [R01814\\_Tph2](#) and as a product in [TRPtrans\\_Slc7a5](#), [TRPtrans\\_Slc7a8](#) and as a modifier in [R00677](#), [R00678\\_Tdo](#), [R00685](#), [R01814\\_Tph1](#), [R02701](#), [R02702](#),

R03664, TRPtrans\_Slc7a5, R00678\_Indo, R02909, R01814\_Tph2, TRPtrans\_Slc7a8, Lkynr-trans\_Slc7a5, Lkynr-trans\_Slc7a8).

$$\frac{d}{dt}M_{\text{trp\_DASH\_L\_c}} = v_{19} + v_{40} - v_1 - v_2 - v_3 - v_5 - v_{14} - v_{20} - v_{39} \quad (108)$$

## 7.25 Species $M_{\text{trp\_L\_trna\_c}}$

**Name** M\_Trp\_tRNA

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

This species takes part in one reaction (as a product in R03664), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{\text{trp\_L\_trna\_c}} = 0 \quad (109)$$

## 7.26 Species $M_{\text{trypta\_c}}$

**Name** M\_Trypta

**Initial concentration**  $3.59090204143853 \cdot 10^{-9} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in 14 reactions (as a reactant in R02174, R02173\_Maoa, R02173\_Maob, AANAT\_Trypta and as a product in R00685 and as a modifier in R02174, R02173\_Maoa, R02908-Maoa, R02911, R02174\_metTrypta, R02910, R02908\_Maob, R02173\_Maob, AANAT\_Trypta).

$$\frac{d}{dt}M_{\text{trypta\_c}} = v_3 - v_9 - v_{17} - v_{37} - v_{38} \quad (110)$$

## 7.27 Species $M_{\text{amp\_c}}$

**Name** M\_AMP

**Initial concentration**  $0.999999951844375 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in R03664), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{\text{amp\_c}} = 0 \quad (111)$$



### 7.28 Species $M_{\text{atp\_c}}$

**Name**  $M_{\text{ATP}}$

**Initial concentration**  $0.999999951844375 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in [R03664](#), [R03005](#) and as a modifier in [R03664](#), [R03005](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{\text{atp\_c}} = 0 \quad (112)$$

### 7.29 Species $M_{\text{co2\_c}}$

**Name**  $M_{\text{CO2}}$

**Initial concentration**  $0.999999951844375 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a product in [R00685](#), [R02701](#), [R03348](#), [R04323](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{\text{co2\_c}} = 0 \quad (113)$$

### 7.30 Species $M_{\text{h2o2\_c}}$

**Name**  $M_{\text{H2O2}}$

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

This species takes part in six reactions (as a product in [R00677](#), [R02173\\_Maoa](#), [R02670](#), [R02908\\_Maoa](#), [R02908\\_Maob](#), [R02173\\_Maob](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{\text{h2o2\_c}} = 0 \quad (114)$$

### 7.31 Species $M_{\text{h2o\_c}}$

**Name**  $M_{\text{H2O}}$

**Initial concentration**  $1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in 15 reactions (as a reactant in [R00677](#), [R00987](#), [R01959](#), [R02668](#), [R04911](#), [R02173\\_Maoa](#), [R03936](#), [R00988](#), [R02908\\_Maoa](#), [R02908\\_Maob](#), [R02173\\_Maob](#) and as a product in [R01814\\_Tph1](#), [R01960](#), [R01814\\_Tph2](#) and as a modifier in [R00677](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{\text{h2o\_c}} = 0 \quad (115)$$

### 7.32 Species $M_{h\_c}$

**Name**  $M_H$

**Initial concentration**  $1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in nine reactions (as a reactant in [R01960](#), [R03348](#), [R03005](#) and as a product in [R02670](#), [R02911](#), [AANAT\\_Trypta](#) and as a modifier in [R01960](#), [R03348](#), [R03005](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{h\_c} = 0 \quad (116)$$

### 7.33 Species $M_{nadp\_c}$

**Name**  $M_{NADP}$

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

This species takes part in one reaction (as a product in [R01960](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{nadp\_c} = 0 \quad (117)$$

### 7.34 Species $M_{nadph\_c}$

**Name**  $M_{NADPH}$

**Initial concentration**  $0.03 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [R01960](#) and as a modifier in [R01960](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{nadph\_c} = 0 \quad (118)$$

### 7.35 Species $M_{nh4\_c}$

**Name**  $M_{NH4}$

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

This species takes part in five reactions (as a product in [R00677](#), [R02173\\_Maoa](#), [R02908\\_Maoa](#), [R02908\\_Maob](#), [R02173\\_Maob](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{nh4\_c} = 0 \quad (119)$$

### 7.36 Species `M_o2_c`

**Name** `M_O2`

**Initial concentration**  $1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in 24 reactions (as a reactant in [R00677](#), [R00678\\_Tdo](#), [R01814\\_Tph1](#), [R01960](#), [R02665](#), [R02702](#), [R02173\\_Maoa](#), [R02670](#), [R00678\\_Indo](#), [R02908\\_Maoa](#), [R02909](#), [R02908-Maob](#), [R02173\\_Maob](#), [R01814\\_Tph2](#) and as a modifier in [R00677](#), [R00678\\_Tdo](#), [R01814\\_Tph1](#), [R01960](#), [R02665](#), [R02702](#), [R02670](#), [R00678\\_Indo](#), [R02909](#), [R01814\\_Tph2](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{o2\_c} = 0 \quad (120)$$

### 7.37 Species `M_o2s_c`

**Name** `M_O2s`

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

This species takes part in one reaction (as a product in [R02670](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{o2s\_c} = 0 \quad (121)$$

### 7.38 Species `M_ppi_c`

**Name** `M_PPi`

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

This species takes part in three reactions (as a product in [R03664](#), [R03348](#), [R03005](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{ppi\_c} = 0 \quad (122)$$

### 7.39 Species `M_Cinnavalininate_c`

**Name** `M_Cin`

**Initial concentration**  $1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R02670](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{Cinnavalininate\_c} = 0 \quad (123)$$

#### 7.40 Species [M\\_kynate\\_c](#)

**Name** M\_Kyna

**Initial concentration** 1 mmol · l<sup>-1</sup>

This species takes part in four reactions (as a product in [R01956\\_Kat1](#), [R04171\\_Kat2](#), [R04171-Kat3](#) and as a modifier in [R04323](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{\text{kynate\_c}} = 0 \quad (124)$$

#### 7.41 Species [TRP\\_ex](#)

**Name** Trp\_ex

**Initial concentration** 0.0050 mmol · l<sup>-1</sup>

This species takes part in six reactions (as a reactant in [TRPtrans\\_Slc7a5](#), [TRPtrans\\_Slc7a8](#) and as a modifier in [TRPtrans\\_Slc7a5](#), [TRPtrans\\_Slc7a8](#), [Lkynr\\_trans\\_Slc7a5](#), [Lkynr-trans\\_Slc7a8](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}TRP_{\text{ex}} = 0 \quad (125)$$

#### 7.42 Species [M\\_nicrnt\\_c](#)

**Name** M\_NaMN

**Initial concentration** 9.50021481464022 · 10<sup>-16</sup> mmol · l<sup>-1</sup>

This species takes part in three reactions (as a reactant in [R03005](#) and as a product in [R03348](#) and as a modifier in [R03005](#)).

$$\frac{d}{dt}M_{\text{nicrnt\_c}} = v_{21} - v_{24} \quad (126)$$

#### 7.43 Species [M\\_prpp\\_c](#)

**Name** M\_PRPP

**Initial concentration** 1 mmol · l<sup>-1</sup>

This species takes part in two reactions (as a reactant in [R03348](#) and as a modifier in [R03348](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{\text{prpp\_c}} = 0 \quad (127)$$

#### 7.44 Species `M_nformanth_c`

**Name** `M_FAA`

**Initial concentration**  $7.14152660211118 \cdot 10^{-9} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [R00988](#) and as a product in [R03936](#) and as a modifier in [R01959](#), [R04911](#), [R00988](#)).

$$\frac{d}{dt}M\_nformanth\_c = v_{22} - v_{23} \quad (128)$$

#### 7.45 Species `M_dnad_c`

**Name** `M_NAAD`

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

This species takes part in one reaction (as a product in [R03005](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_dnad\_c = 0 \quad (129)$$

#### 7.46 Species `M_am6sa_c`

**Name** `M_Am6sa`

**Initial concentration**  $1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R04323](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_am6sa\_c = 0 \quad (130)$$

#### 7.47 Species `M_5hoxindact_c`

**Name** `M_5HAc`

**Initial concentration**  $1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a product in [R02908\\_Maoa](#), [R02908\\_Maob](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_5hoxindact\_c = 0 \quad (131)$$

#### 7.48 Species `M_Nacsertn_c`

**Name** `M_NAcSet`

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

This species takes part in one reaction (as a product in [R02911](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_Nacsertn\_c = 0 \quad (132)$$

#### 7.49 Species `M_accoa_c`

**Name** `M_AcetylCoA`

**Initial concentration**  $0.999999951844375 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [R02911](#), [AANAT\\_Trypta](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_accoa\_c = 0 \quad (133)$$

#### 7.50 Species `M_coa_c`

**Name** `M_CoA`

**Initial concentration**  $1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a product in [R02911](#), [AANAT\\_Trypta](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_coa\_c = 0 \quad (134)$$

#### 7.51 Species `M_Xanthurenate`

**Name** `M_Xanth`

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

This species takes part in three reactions (as a product in [R04171\\_Kat1](#), [R01956\\_Kat2](#), [R01956-Kat3](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M\_Xanthurenate = 0 \quad (135)$$

### 7.52 Species [M\\_f5hoxkyn\\_c](#)

**Name** M\_F5HKyn

**Initial concentration** 0 mmol · l<sup>-1</sup>

This species takes part in one reaction (as a product in [R02909](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{f5hoxkyn\_c} = 0 \quad (136)$$

### 7.53 Species [M\\_nndmtrpta\\_c](#)

**Name** M\_MMTrypta

**Initial concentration** 0 mmol · l<sup>-1</sup>

This species takes part in one reaction (as a product in [R02174\\_metTrypta](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{nndmtrpta\_c} = 0 \quad (137)$$

### 7.54 Species [M\\_nmsrtn\\_c](#)

**Name** M\_NMSer

**Initial concentration** 0 mmol · l<sup>-1</sup>

This species takes part in one reaction (as a product in [R02910](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}M_{nmsrtn\_c} = 0 \quad (138)$$

### 7.55 Species [M\\_Nactrypta\\_c](#)

**Name** M\_Nactrypta

**Initial concentration** 0 mmol · l<sup>-1</sup>

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

$$\frac{d}{dt}M_{Nactrypta\_c} = 0 \quad (139)$$

## 7.56 Species `M_Lkynr_ex`

**Name** `M_LKyn_ex`

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

This species takes part in six reactions (as a product in `Lkynr_trans_Slc7a5`, `Lkynr_trans_Slc7a8` and as a modifier in `TRPtrans_Slc7a5`, `TRPtrans_Slc7a8`, `Lkynr_trans_Slc7a5`, `Lkynr_trans_Slc7a8`), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} M\_Lkynr\_ex = 0 \quad (140)$$

SBML2<sup>AT</sup>EX was developed by Andreas Dräger<sup>a</sup>, Hannes Planatscher<sup>a</sup>, Dieudonné M Wouamba<sup>a</sup>, Adrian Schröder<sup>a</sup>, Michael Hucka<sup>b</sup>, Lukas Endler<sup>c</sup>, Martin Golebiewski<sup>d</sup> and Andreas Zell<sup>a</sup>. Please see <http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX> for more information.

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