SBML Model Report

Model name: "Winter2017 - Brain Energy Metabolism with PPP"

March 2, 2017

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by Felix Winter[1] at July 30th 2013 at 11:50 a. m. and last time modified at October 22nd 2014 at 9:29 a. m. Table 1 shows an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	6
species types	0	species	65
events	0	constraints	0
reactions	64	function definitions	20
global parameters	103	unit definitions	2
rules	23	initial assignments	18

Model Notes

Winter2017 - Brain Energy Metabolism with PPP

This model is described in the article:Mathematical analysis of the influence of brain metabolism on the BOLD signal in Alzheimer's diseaseFelix Winter1,2, Catrin Bludszuweit-Philipp1 and Olaf Wolkenhauer2,3Journal of Cerebral Blood Flow & Metabolism

Abstract:

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Blood oxygen level-dependent functional magnetic resonance imaging (BOLD-fMRI) is a standard clinical tool for the detection of brain activation. In Alzheimers disease (AD), task-related and resting state fMRI have been used to detect brain dysfunction. It has been shown that the shape of the BOLD response is affected in early AD. To correctly interpret these changes, the mechanisms responsible for the observed behaviour need to be known. The parameters of the canonical hemodynamic response function (HRF) commonly used in the analysis of fMRI data have no direct biological interpretation and cannot be used to answer this question. We here present a model that allows relating AD-specific changes in the BOLD shape to changes in the underlying energy metabolism. According to our findings, the classic view that differences in the BOLD shape are only attributed to changes in strength and duration of the stimulus does not hold. Instead, peak height, peak timing and full width at half maximum are sensitive to changes in the reaction rate of several metabolic reactions. Our systems-theoretic approach allows the use of patient-specific clinical data to predict dementia- driven changes in the HRF, which can be used to improve the results of fMRI analyses in AD patients.

This model is hosted on BioModels Database and identified by: BIOMD0000000627.

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

2 Unit Definitions

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

2.1 Unit `volume`

Name volume

Definition ml

2.2 Unit `substance`

Name substance

Definition mmol

2.3 Unit `area`

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

Definition m^2

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 Compartments

This model contains six compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment_1	capillary	0000290	3	0.0055	ml	☑	
compartment_2	neurons	0000290	3	0.45	ml	☑	
compartment_3	astrocytes	0000290	3	0.25	ml	☑	
compartment_4	extracellular_space	0000290	3	0.2	ml	☑	
venous_balloon	venous balloon	0000290	3	0.0237	ml	☐	
artery	artery	0000290	3	0.0055	ml	☑	

3.1 Compartment compartment_1

This is a three dimensional compartment with a constant size of 0.0055 ml.

Name capillary

SBO:0000290 physical compartment

3.2 Compartment compartment_2

This is a three dimensional compartment with a constant size of 0.45 ml.

Name neurons

SBO:0000290 physical compartment

3.3 Compartment compartment_3

This is a three dimensional compartment with a constant size of 0.25 ml.

Name astrocytes

SBO:0000290 physical compartment

3.4 Compartment `compartment_4`

This is a three dimensional compartment with a constant size of 0.2 ml.

Name extracellular_space

SBO:0000290 physical compartment

3.5 Compartment `venous_balloon`

This is a three dimensional compartment with a not constant size of 0.0237 ml.

Name venous balloon

SBO:0000290 physical compartment

3.6 Compartment `artery`

This is a three dimensional compartment with a constant size of 0.0055 ml.

Name artery

SBO:0000290 physical compartment

4 Species

This model contains 65 species. The boundary condition of five of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 10 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
species_23	O2	compartment_1	mmol	⊟	⊟
species_24	CO2	compartment_1	mmol	⊟	⊟
species_25	GLC	compartment_1	mmol	⊟	⊟
species_26	LAC	compartment_1	mmol	⊟	⊟
dHb	dHb	compartment_1	mmol	⊟	⊟
species_1	GLC	compartment_2	mmol	⊟	⊟
species_2	G6P	compartment_2	mmol	⊟	⊟
species_3	ATP	compartment_2	mmol	⊟	⊟
species_7	F6P	compartment_2	mmol	⊟	⊟
species_9	GAP	compartment_2	mmol	⊟	⊟
species_11	NADH	compartment_2	mmol	⊟	⊟
species_12	PEP	compartment_2	mmol	⊟	⊟
species_15	PYR	compartment_2	mmol	⊟	⊟
species_18	LAC	compartment_2	mmol	⊟	⊟
species_16	O2	compartment_2	mmol	⊟	⊟
species_21	PCr	compartment_2	mmol	⊟	⊟
Na__neurons	Na+	compartment_2	mmol	⊟	⊟
GLU_neurons	GLU	compartment_2	mmol	⊟	⊟
ADP_neurons	ADP	compartment_2	mmol	⊟	⊟
AMP_neurons	AMP	compartment_2	mmol	⊟	⊟
Cr_neurons	Cr	compartment_2	mmol	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
NAD_neurons	NAD	compartment_2	mmol	⊟	⊟
G6L_neurons	G6L	compartment_2	mmol	⊟	⊟
P6G_neurons	P6G	compartment_2	mmol	⊟	⊟
Ru5P_neurons	Ru5P	compartment_2	mmol	⊟	⊟
X5P_neurons	X5P	compartment_2	mmol	⊟	⊟
R5P_neurons	R5P	compartment_2	mmol	⊟	⊟
S7P_neurons	S7P	compartment_2	mmol	⊟	⊟
E4P_neurons	E4P	compartment_2	mmol	⊟	⊟
NADPH_neurons	NADPH	compartment_2	mmol	⊟	⊟
NADP_neurons	NADP	compartment_2	mmol	⊟	⊟
species_4	GLC	compartment_3	mmol	⊟	⊟
species_5	ATP	compartment_3	mmol	⊟	⊟
species_6	G6P	compartment_3	mmol	⊟	⊟
species_8	F6P	compartment_3	mmol	⊟	⊟
species_10	GAP	compartment_3	mmol	⊟	⊟
species_13	NADH	compartment_3	mmol	⊟	⊟
species_14	PEP	compartment_3	mmol	⊟	⊟
species_17	PYR	compartment_3	mmol	⊟	⊟
species_19	LAC	compartment_3	mmol	⊟	⊟
species_20	O2	compartment_3	mmol	⊟	⊟
species_22	PCr	compartment_3	mmol	⊟	⊟
Na__astrocytes	Na+	compartment_3	mmol	⊟	⊟
GLU_astrocytes	GLU	compartment_3	mmol	⊟	⊟
ADP_astrocytes	ADP	compartment_3	mmol	⊟	⊟
AMP_astrocytes	AMP	compartment_3	mmol	⊟	⊟
Cr_astrocytes	Cr	compartment_3	mmol	⊟	⊟
NAD_astrocytes	NAD	compartment_3	mmol	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
G6L_astrocytes	G6L	compartment_3	mmol	⊟	⊟
P6G_astrocytes	P6G	compartment_3	mmol	⊟	⊟
Ru5P_astrocytes	Ru5P	compartment_3	mmol	⊟	⊟
X5P_astrocytes	X5P	compartment_3	mmol	⊟	⊟
R5P_astrocytes	R5P	compartment_3	mmol	⊟	⊟
S7P_astrocytes	S7P	compartment_3	mmol	⊟	⊟
E4P_astrocytes	E4P	compartment_3	mmol	⊟	⊟
NADP_astrocytes	NADP	compartment_3	mmol	⊟	⊟
NADPH_astrocytes	NADPH	compartment_3	mmol	⊟	⊟
species_27	GLC	compartment_4	mmol	⊟	⊟
species_28	LAC	compartment_4	mmol	⊟	⊟
GLU_extracellular_space	GLU	compartment_4	mmol	⊟	⊟
Na_extracellular_space	Na+	compartment_4	mmol	☑	☑
O2_artery	O2	artery	mmol	☑	☑
CO2_artery	CO2	artery	mmol	☑	☑
GLC_artery	GLC	artery	mmol	☑	☑
LAC_artery	LAC	artery	mmol	☑	☑

5 Parameters

This model contains 103 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
parameter_1	K_m_GLC		0.105		☑
parameter_2	K_m_G6P		0.500		☑
parameter_3	K_m_F6P_PGI		0.060		☑
parameter_4	K_m_F6P_PFK		0.180		☑
parameter_5	K_I_ATP		1.000		☑
parameter_6	nH		4.000		☑
parameter_7	NADH_total-_neurons		0.220		☑
parameter_8	NADH_total-_astrocytes		0.220		☑
parameter_9	NAD_neurons		0.204		⊟
parameter_10	NAD_astrocytes		0.162		⊟
parameter_11	ANP		2.379		☑
parameter_12	q_AK		0.920		☑
parameter_14	K_m_ATP		0.015		☑
parameter_16	K_m_ADP		0.001		☑
parameter_17	K_m_O2		0.003		☑
parameter_18	K_m_PYR		0.063		☑
parameter_19	PCr_total		5.000		☑
parameter_20	Cr_neurons		3.559		⊟
parameter_21	Cr_astrocytes		4.623		⊟
parameter_25	Vmax_ATPase-_neurons		0.049		☑
parameter_26	Vmax_ATPase-_astrocytes		0.036		☑
parameter_43	Vmax_ec_LAC (wrt extracellular space)		0.033		☑
F_0	F_0		0.012		☑
delta_F	delta_F		0.420		☑
t_0	t_0		200.000		☑
t_end	t_end		40.000		☑
t_1	t_1		2.000		☑
F_in	F_in		0.012		⊟
F_out	F_out		0.012		⊟
tau_v	tau_v		35.000		☑
Hb_OP	Hb.OP		8.600		☑

Id	Name	SBO	Value	Unit	Constant
Sm_g	Sm_g		10500.000		☑
Sm_n	Sm_n		40500.000		☑
k_pump	k_pump		$3.17 \cdot 10^{-7}$		☑
K_m_Na_pump	K_m,Na-pump		0.424		☑
K_m_G6P_GLYS	K_m_G6P_GLYS		0.500		☑
delta_GLY	delta_GLY		62.000		☑
K_m_GLY	K_m_GLY		1.000		☑
g_Na_neurons	g_Na_neurons		0.004		☑
g_Na-_astrocytes	g_Na_astrocytes		0.003		☑
Vm	Vm		−70.000		☑
RT	RT		2577340.000		☑
F	F		96500.000		☑
vn_1_tp	vn_1		0.041		☑
vn_2_tp	vn_2		1.440		☑
t_stim_tp	t_stim_tp		2.000		☑
is-_stimulated	is_stimulated		0.000		⊟
v_stim	v_stim		0.000		⊟
R_Na_GLU	R_Na_GLU		0.075		☑
V_eg_max_GLU	V_eg_max_GLU		0.021		☑
K_m_GLU	K_m_GLU		0.050		☑
V_gn_max_GLU	V_gn_max_GLU		0.300		☑
delta_HK	delta_HK		0.600		☑
BOLD_signal	BOLD signal		0.000		⊟
E0	E0		0.242		⊟
K_m_ATP-_ATPase	K_m_ATP(ATPase)		0.001		☑
NULL	NULL		0.000		☑
Vmax_ne-_LAC__wrt-_extracellular-_space	Vmax_ne_LAC (wrt extracellular space)		0.445		☑
PS_cap-_astrocytes-__wrt-_capillaries	PS_cap_astrocytes (wrt capillaries)		11.162		☑
PS_cap-_neuron__wrt-_capillaries	PS_cap_neuron (wrt capillaries)		18.016		☑

Id	Name	SBO	Value	Unit	Constant
Vmax_eg_GLU__wrt_extracellular_space	Vmax_eg_GLU (wrt extracellular space)		0.026		☑
K_T_GLC_ce__Aubert	K_T_GLC_ce (Aubert)		9.000		☑
Vmax_ce_GLC__wrt_capillaries___Aubert	Vmax_ce_GLC (wrt capillaries) (Aubert)		4.291		⊟
Vmax_eg_GLC__wrt_astrocytes___Aubert_	Vmax_eg_GLC (wrt astrocytes) (Aubert)		1275.000		⊟
K_T_GLC_eg__Aubert	K_T_GLC_eg (Aubert)		9.000		☑
K_T_GLC_en__Aubert	K_T_GLC_en (Aubert)		9.000		☑
Vmax_en_GLC__wrt_neurons___Aubert	Vmax_en_GLC (wrt neurons) (Aubert)		11767.500		⊟
K_T_GLC_cg__Aubert	K_T_GLC_cg (Aubert)		9.000		☑
Vmax_cg_GLC__wrt_capillaries___Aubert	Vmax_cg_GLC (wrt capillaries) (Aubert)		0.423		⊟
Vmax_ec_LAC__wrt_extracellular_space__Aubert	Vmax_ec_LAC (wrt extracellular space) (Aubert)		0.006		⊟
Vmax_gc_LAC__wrt_astrocytes___Aubert	Vmax_gc_LAC (wrt astrocytes) (Aubert)		0.004		⊟
Vmax_ge_LAC__wrt_astrocytes___Aubert	Vmax_ge_LAC (wrt astrocytes) (Aubert)		0.057		⊟

Id	Name	SBO	Value	Unit	Constant
Vmax_ne_LAC_-_wrt_neurons-__Aubert	Vmax_ne_LAC (wrt neurons) (Aubert)		0.218		⊟
K_T_LAC_ne_-_Aubert	K_T_LAC_ne (Aubert)		0.500		☑
K_T_LAC_ge_-_Aubert	K_T_LAC_ge (Aubert)		0.500		☑
K_T_LAC_gc_-_Aubert	K_T_LAC_gc (Aubert)		0.500		☑
K_T_LAC_ec_-_Aubert	K_T_LAC_ec (Aubert)		0.500		☑
PS_cap-_astrocytes-__wrt-_capillaries-__Aubert	PS_cap_astrocytes (wrt capillaries) (Aubert)		4.705		⊟
PS_cap-_neuron__wrt-_capillaries-__Aubert	PS_cap_neuron (wrt capillaries) (Aubert)		40.500		⊟
K_O2__Aubert	K_O2 (Aubert)		0.036		☑
nh_O2__Aubert	nh_O2 (Aubert)		2.730		☑
Vmax_f_PGI_-_Cloutier	Vmax_f_PGI (Cloutier)		0.500		☑
Vmax_r_PGI_-_Cloutier	Vmax_r_PGI (Cloutier)		0.450		☑
Vmax_ce_GLC_-_Aubert	Vmax_ce_GLC (Aubert)		0.118		☑
Vmax_cg_GLC_-__Aubert	Vmax_cg_GLC (Aubert)		0.009		☑
Vmax_eg_GLC_-_Aubert_	Vmax_eg_GLC (Aubert)		1020.000		☑
Vmax_en_GLC_-__Aubert	Vmax_en_GLC (Aubert)		5230.000		☑
_sf	sf		0.750		☑
_PScap	_PScap		1.100		☑
f_CBF_dyn	f_CBF_dyn		1.000		⊟
stimulus	stimulus		$-3.87088868421524 \cdot 10^{45}$		⊟
Metabolite-_123	Initial for O2		8.340		☑
Metabolite_1	Initial for O2		7.332		☑
Metabolite_9	Initial for dHb		0.048		☑

Id	Name	SBO	Value	Unit	Constant
Compartment_9	Initial for venous balloon		0.024		☑
ModelValue_54	Initial for E0		0.242		☑
ModelValue_7	Initial for NADH_total_astrocytes		0.220		☑
ModelValue_6	Initial for NADH_total_neurons		0.220		☑
ModelValue_16	Initial for PCr_total		5.000		☑
ModelValue_83	Initial for Vmax_ce_GLC (Aubert)		0.118		☑
ModelValue_84	Initial for Vmax_cg_GLC (Aubert)		0.009		☑
ModelValue_86	Initial for Vmax_en_GLC (Aubert)		5230.000		☑
ModelValue_43	Initial for vn_1		0.041		☑

6 Initialassignments

This is an overview of 18 initialassignments.

6.1 Initialassignment AMP_neurons

Derived unit contains undeclared units

Math $\left(\text{parameter\_11} - \frac{\text{ADP\_neurons}}{\text{vol(compartment\_2)}} - \frac{\text{species\_3}}{\text{vol(compartment\_2)}}\right) \cdot \text{vol}\left(\text{compartment\_2}\right)$

6.2 Initialassignment Cr_neurons

Derived unit contains undeclared units

Math $\left(\text{parameter\_19} - \frac{\text{species\_21}}{\text{vol(compartment\_2)}}\right) \cdot \text{vol}\left(\text{compartment\_2}\right)$

6.3 Initialassignment NAD_neurons

Derived unit contains undeclared units

Math $\left(\text{parameter\_7} - \frac{\text{species\_11}}{\text{vol(compartment\_2)}}\right) \cdot \text{vol}\left(\text{compartment\_2}\right)$

6.4 Initialassignment AMP_astrocytes

Derived unit contains undeclared units

Math $\left(\text{parameter\_11} - \frac{\text{ADP\_astrocytes}}{\text{vol}(\text{compartment\_3})} - \frac{\text{species\_5}}{\text{vol}(\text{compartment\_3})}\right) \cdot \text{vol}\left(\text{compartment\_3}\right)$

6.5 Initialassignment Cr_astrocytes

Derived unit contains undeclared units

Math $\left(\text{parameter\_19} - \frac{\text{species\_22}}{\text{vol}(\text{compartment\_3})}\right) \cdot \text{vol}\left(\text{compartment\_3}\right)$

6.6 Initialassignment NAD_astrocytes

Derived unit contains undeclared units

Math $\left(\text{parameter\_8} - \frac{\text{species\_13}}{\text{vol}(\text{compartment\_3})}\right) \cdot \text{vol}\left(\text{compartment\_3}\right)$

6.7 Initialassignment Metabolite_123

Derived unit mmol

Math O2_artery

6.8 Initialassignment Metabolite_1

Derived unit mmol

Math species_23

6.9 Initialassignment Metabolite_9

Derived unit mmol

Math dHb

6.10 Initialassignment Compartment_9

Derived unit ml

Math $\text{vol}\left(\text{venous\_balloon}\right)$

6.11 Initialassignment ModelValue_54

Derived unit contains undeclared units

Math E0

6.12 Initialassignment ModelValue_7

Derived unit contains undeclared units

Math parameter_8

6.13 Initialassignment ModelValue_6

Derived unit contains undeclared units

Math parameter_7

6.14 Initialassignment ModelValue_16

Derived unit contains undeclared units

Math parameter_19

6.15 Initialassignment ModelValue_83

Derived unit contains undeclared units

Math Vmax_ce_GLC__Aubert

6.16 Initialassignment ModelValue_84

Derived unit contains undeclared units

Math Vmax_cg_GLC___Aubert

6.17 Initialassignment ModelValue_86

Derived unit contains undeclared units

Math Vmax_en_GLC___Aubert

6.18 Initialassignment ModelValue_43

Derived unit contains undeclared units

Math vn_1_tp

7 Function definitions

This is an overview of 20 function definitions.

7.1 Function definition vdHb_in

Name vdHb_in [1]

Arguments F_in, O2_a, O2_c

Mathematical Expression

$$\mathrm{F\_in} \cdot (\mathrm{O2\_a} - 2 \cdot \mathrm{O2\_c} - \mathrm{O2\_a}) \tag{1}$$

7.2 Function definition vdHb_out

Name vdHb_out

Arguments F_out, dHb, V_v

Mathematical Expression

$$\frac{\mathrm{F\_out} \cdot \mathrm{dHb}}{\mathrm{V\_v}} \tag{2}$$

7.3 Function definition vATPase

Name vATPase

Arguments VmaxATPase, ATP, Km_ATP

Mathematical Expression

$$\mathrm{VmaxATPase} \cdot \frac{\mathrm{ATP}}{\mathrm{ATP} + \mathrm{Km\_ATP}} \tag{3}$$

7.4 Function definition vPK

Name vPK

Arguments k_PK, PEP, ADP

Mathematical Expression

$$\mathrm{k\_PK} \cdot \mathrm{PEP} \cdot \mathrm{ADP} \tag{4}$$

7.5 Function definition vPGK

Name vPGK

Arguments k_PGK, GAP, ADP, NAD, NADH

Mathematical Expression

$$\mathrm{k\_PGK} \cdot \mathrm{GAP} \cdot \mathrm{ADP} \cdot \frac{\mathrm{NAD}}{\mathrm{NADH}} \tag{5}$$

7.6 Function definition vPFK

Name vPFK

Arguments k_PFK, ATP, K_I_ATP, nH, F6P, K_m_F6P

Mathematical Expression

$$\mathrm{k\_PFK} \cdot \mathrm{ATP} \cdot \left(1 + \left(\frac{\mathrm{ATP}}{\mathrm{K\_I\_ATP}}\right)^{\mathrm{nH}}\right)^{1} \cdot \frac{\mathrm{F6P}}{\mathrm{F6P} + \mathrm{K\_m\_F6P}} \tag{6}$$

7.7 Function definition facilitated_transport__inkl__Volume

Name facilitated transport (inkl. Volume)

Arguments Vmax, S, K, P, Volume

Mathematical Expression

$$\mathrm{Vmax} \cdot \left(\frac{\mathrm{S}}{\mathrm{S} + \mathrm{K}} - \frac{\mathrm{P}}{\mathrm{P} + \mathrm{K}}\right) \cdot \mathrm{Volume} \tag{7}$$

7.8 Function definition vGLU_eg__inkl__Volumes

Name vGLU_eg (inkl. Volumes)

Arguments Vmax_GLU, GLU_e, K_m_GLU, Volume

Mathematical Expression

$$\mathrm{Vmax\_GLU} \cdot \frac{\mathrm{GLU\_e}}{\mathrm{GLU\_e} + \mathrm{K\_m\_GLU}} \cdot \mathrm{Volume} \tag{8}$$

7.9 Function definition vGLU_gn__inkl__Volume

Name vGLU_gn (inkl. Volume)

Arguments Vmax_GLU, GLU_g, K_m_GLU, ATP_g, K_m_ATP, Volume

Mathematical Expression

$$\mathrm{Vmax\_GLU} \cdot \frac{\mathrm{GLU\_g}}{\mathrm{GLU\_g} + \mathrm{K\_m\_GLU}} \cdot \frac{\mathrm{ATP\_g}}{\mathrm{ATP\_g} + \mathrm{K\_m\_ATP}} \cdot \mathrm{Volume} \tag{9}$$

7.10 Function definition vGLU_ne__inkl__Volume

Name vGLU_ne (inkl. Volume)

Arguments vSTIM, ratio_Na_GLU, GLU_n, Km_GLU, Volume

Mathematical Expression

$$\text{vSTIM} \cdot \text{ratio\_Na\_GLU} \cdot \frac{\text{GLU\_n}}{\text{GLU\_n} + \text{Km\_GLU}} \cdot \text{Volume} \tag{10}$$

7.11 Function definition vStim__with_volume

Name vStim (with volume)

Arguments vstim, Volume

Mathematical Expression

$$\text{vstim} \cdot \text{Volume} \tag{11}$$

7.12 Function definition modular_rate_law_for_two_substrates__two_products

Name modular rate law for two substrates, two products

Arguments Vmax, K_S1, K_S2, S1, S2, P1, P2, Keq, K_P1, K_P2

Mathematical Expression

$$\text{Vmax} \cdot \frac{1}{\text{K\_S1} \cdot \text{K\_S2}} \cdot \frac{\text{S1} \cdot \text{S2} - \frac{\text{P1} \cdot \text{P2}}{\text{Keq}}}{\left(1 + \frac{\text{S1}}{\text{K\_S1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{K\_S2}}\right) + \left(1 + \frac{\text{P1}}{\text{K\_P1}}\right) \cdot \left(1 + \frac{\text{P2}}{\text{K\_P2}}\right) - 1} \tag{12}$$

7.13 Function definition modular_rate_law_for_one_substrate__one_product

Name modular rate law for one substrate, one product

Arguments Vmax, K_S1, S1, P1, Keq, K_P1

Mathematical Expression

$$\text{Vmax} \cdot \frac{1}{\text{K\_S1}} \cdot \frac{\text{S1} - \frac{\text{P1}}{\text{Keq}}}{1 + \frac{\text{S1}}{\text{K\_S1}} + 1 + \frac{\text{P1}}{\text{K\_P1}} - 1} \tag{13}$$

7.14 Function definition Blood_flow_contribution_inkl__volume

Name Blood flow contribution inkl. volume

Arguments F_in, V_c, Volume, Substrate, Product

Mathematical Expression

$$\frac{2 \cdot \text{F\_in}}{\text{V\_c}} \cdot (\text{Substrate} - \text{Product}) \cdot \text{Volume} \tag{14}$$

7.15 Function definition O2_transport_function_inkl__volume

Name O2 transport function inkl. volume

Arguments PScap, Volume, KO2, HbOP, O2_source, nh, O2_destination, Volume1

Mathematical Expression

$$\frac{\text{PScap}}{\text{Volume}} \cdot \left(\text{KO2} \cdot \left(\frac{\text{HbOP}}{\text{O2\_source}} - 1 \right)^{\frac{1}{\text{nh}}} - \text{O2\_destination} \right) \cdot \text{Volume1} \tag{15}$$

7.16 Function definition vLEAK_Na_inkl__Volume

Name vLEAK_Na inkl. Volume

Arguments Sm, gNA, Volume, F, RT, Na_e, Na, Vm, Volume1

Mathematical Expression

$$\frac{\text{Sm} \cdot \text{gNA}}{\text{Volume} \cdot \text{F}} \cdot \left(\frac{\text{RT}}{\text{F}} \cdot \left(\frac{\text{Na\_e}}{\text{Na}} \right) - \text{Vm} \right) \cdot \text{Volume1} \tag{16}$$

7.17 Function definition vPUMP_volume_dependent

Name vPUMP volume dependent

Arguments Sm, Volume, k_pump, ATP, Na, Km_pump

Mathematical Expression

$$\frac{\text{Sm}}{\text{Volume}} \cdot \text{k\_pump} \cdot \text{ATP} \cdot \text{Na} \cdot \left(1 + \frac{\text{ATP}}{\text{Km\_pump}} \right)^{1} \tag{17}$$

7.18 Function definition vHK__HS

Name vHK (HS)

Arguments k_HK, ATP, G6P, K_I_G6P

Mathematical Expression

$$\mathrm{k\_HK} \cdot \mathrm{ATP} \cdot \left(1 + \frac{\mathrm{G6P}}{\mathrm{K\_I\_G6P}}\right)^{1} \tag{18}$$

7.19 Function definition facilitated_transport__inkl__Volume____scaled

Name facilitated transport (inkl. Volume) (scaled)

Arguments Vmax, sf, S, K, P, Volume

Mathematical Expression

$$\mathrm{Vmax} \cdot \mathrm{sf} \cdot \left(\frac{\mathrm{S}}{\mathrm{S} + \mathrm{K}} - \frac{\mathrm{P}}{\mathrm{P} + \mathrm{K}}\right) \cdot \mathrm{Volume} \tag{19}$$

7.20 Function definition vMITO2__inkl__Volumes

Name vMITO2 (inkl. Volumes)

Arguments v_max_mito, PYR, K_m_PYR, ADP, K_m_ADP, O2, K_m_O2, alpha, ATP, beta, Volume

Mathematical Expression

$$\begin{aligned} &\mathrm{v\_max\_mito} \cdot \frac{\mathrm{PYR}}{\mathrm{PYR} + \mathrm{K\_m\_PYR}} \cdot \frac{\mathrm{ADP}}{\mathrm{ADP} + \mathrm{K\_m\_ADP}} \\ &\cdot \frac{\mathrm{O2}}{\mathrm{O2} + \mathrm{K\_m\_O2}} \cdot \left(1 - \frac{1}{1 + \exp\left(\mathrm{alpha} \cdot \left(\frac{\mathrm{ATP}}{\mathrm{ADP}} - \mathrm{beta}\right)\right)}\right) \cdot \mathrm{Volume} \end{aligned} \tag{20}$$

8 Rules

This is an overview of 23 rules.

8.1 Rule E0

Rule E0 is an assignment rule for parameter E0:

$$\mathrm{E0} = 1 - \frac{2 \cdot \mathrm{Metabolite\_1} - \mathrm{Metabolite\_123}}{\frac{\mathrm{O2\_artery}}{\mathrm{vol(artery)}}} \tag{21}$$

8.2 Rule BOLD_signal

Rule BOLD_signal is an assignment rule for parameter BOLD_signal:

$$\begin{aligned}\text{BOLD\_signal} = \text{Compartment\_9} \cdot 7 \cdot \left(1 - \frac{\frac{\text{dHb}}{\text{vol(compartment\_1)}}}{\text{Metabolite\_9}}\right) + 2 \cdot \frac{1 - \frac{\frac{\text{dHb}}{\text{vol(compartment\_1)}}}{\text{Metabolite\_9}}}{\frac{\text{vol(venous\_balloon)}}{\text{Compartment\_9}}} \\ + (2 \cdot \text{ModelValue\_54} - 0.2) \cdot \left(1 - \frac{\text{vol}\,(\text{venous\_balloon})}{\text{Compartment\_9}}\right)\end{aligned} \tag{22}$$

8.3 Rule Vmax_ce_GLC__wrt_capillaries___Aubert

Rule Vmax_ce_GLC__wrt_capillaries___Aubert is an assignment rule for parameter Vmax_ce_GLC__wrt_capillaries___Aubert:

$$\text{Vmax\_ce\_GLC\_\_wrt\_capillaries\_\_\_Aubert} = \text{ModelValue\_83} \cdot \frac{\text{vol}\,(\text{compartment\_4})}{\text{vol}\,(\text{compartment\_1})} \tag{23}$$

8.4 Rule Vmax_eg_GLC__wrt_astrocytes___Aubert_

Rule Vmax_eg_GLC__wrt_astrocytes___Aubert_ is an assignment rule for parameter Vmax_eg_GLC__wrt_astrocytes___Aubert_:

$$\text{Vmax\_eg\_GLC\_\_wrt\_astrocytes\_\_\_Aubert\_} = \text{Vmax\_eg\_GLC\_\_Aubert\_} \cdot \frac{\text{vol}\,(\text{compartment\_3})}{\text{vol}\,(\text{compartment\_4})} \tag{24}$$

8.5 Rule Vmax_en_GLC__wrt_neurons___Aubert

Rule Vmax_en_GLC__wrt_neurons___Aubert is an assignment rule for parameter Vmax_en_GLC__wrt_neurons___Aubert:

$$\text{Vmax\_en\_GLC\_\_wrt\_neurons\_\_\_Aubert} = \text{ModelValue\_86} \cdot \frac{\text{vol}\,(\text{compartment\_2})}{\text{vol}\,(\text{compartment\_4})} \tag{25}$$

8.6 Rule Vmax_cg_GLC__wrt_capillaries___Aubert

Rule Vmax_cg_GLC__wrt_capillaries___Aubert is an assignment rule for parameter Vmax_cg_GLC__wrt_capillaries___Aubert:

$$\text{Vmax\_cg\_GLC\_\_wrt\_capillaries\_\_\_Aubert} = \text{ModelValue\_84} \cdot \frac{\text{vol}\,(\text{compartment\_3})}{\text{vol}\,(\text{compartment\_1})} \tag{26}$$

8.7 Rule Vmax_ec_LAC__wrt_extracellular_space___Aubert

Rule Vmax_ec_LAC__wrt_extracellular_space___Aubert is an assignment rule for parameter Vmax_ec_LAC__wrt_extracellular_space___Aubert:

$$\text{Vmax\_ec\_LAC\_\_wrt\_extracellular\_space\_\_\_Aubert} = 0.00783 \cdot \text{\_sf} \tag{27}$$

8.8 Rule Vmax_gc_LAC__wrt_astrocytes___Aubert

Rule Vmax_gc_LAC__wrt_astrocytes___Aubert is an assignment rule for parameter Vmax_gc_LAC__wrt_astrocytes___Aubert:

$$\text{Vmax\_gc\_LAC\_\_wrt\_astrocytes\_\_\_Aubert} = 0.0058 \cdot \text{\_sf} \tag{28}$$

8.9 Rule Vmax_ge_LAC__wrt_astrocytes___Aubert

Rule Vmax_ge_LAC__wrt_astrocytes___Aubert is an assignment rule for parameter Vmax_ge_LAC__wrt_astrocytes___Aubert:

$$\text{Vmax\_ge\_LAC\_\_wrt\_astrocytes\_\_\_Aubert} = 0.076 \cdot \text{\_sf} \tag{29}$$

8.10 Rule Vmax_ne_LAC__wrt_neurons___Aubert

Rule Vmax_ne_LAC__wrt_neurons___Aubert is an assignment rule for parameter Vmax_ne_LAC__wrt_neurons___Aubert:

$$\text{Vmax\_ne\_LAC\_\_wrt\_neurons\_\_\_Aubert} = 0.29 \cdot \text{\_sf} \tag{30}$$

8.11 Rule PS_cap_astrocytes__wrt_capillaries___Aubert

Rule PS_cap_astrocytes__wrt_capillaries___Aubert is an assignment rule for parameter PS_cap_astrocytes__wrt_capillaries___Aubert:

$$\text{PS\_cap\_astrocytes\_\_wrt\_capillaries\_\_\_Aubert} = 0.414 \cdot 0.25 \cdot \frac{\text{vol}\left(\text{compartment\_3}\right)}{\text{vol}\left(\text{compartment\_1}\right)} \tag{31}$$

8.12 Rule PS_cap_neuron__wrt_capillaries___Aubert

Rule PS_cap_neuron__wrt_capillaries___Aubert is an assignment rule for parameter PS_cap_neuron__wrt_capillaries___Aubert:

$$\text{PS\_cap\_neuron\_\_wrt\_capillaries\_\_\_Aubert} = \text{\_PScap} \cdot 0.45 \cdot \frac{\text{vol}\left(\text{compartment\_2}\right)}{\text{vol}\left(\text{compartment\_1}\right)} \tag{32}$$

8.13 Rule f_CBF_dyn

Rule f_CBF_dyn is an assignment rule for parameter f_CBF_dyn:

$$\begin{aligned}\text{f\_CBF\_dyn} = 1 + \text{delta\_F} \cdot \Bigg(& \frac{1}{1 + \exp\left(4.59186 \cdot \left(\text{time} - \text{t\_0} + \text{t\_1} - 3\right)\right)} \\ & - \frac{1}{1 + \exp\left(4.59186 \cdot \left(\text{time} - \left(\text{t\_0} + \text{t\_1} + \text{t\_end} + 3\right)\right)\right)} \Bigg)\end{aligned} \tag{33}$$

8.14 Rule `stimulus`

Rule `stimulus` is an assignment rule for parameter `stimulus`:

$$\text{stimulus} = \text{ModelValue\_43} + \text{vn\_2\_tp} \cdot \frac{\text{time} - \text{t\_0}}{\text{t\_stim\_tp}} \cdot \exp\left(\frac{(\text{time} - \text{t\_0})}{\text{t\_stim\_tp}}\right) \tag{34}$$

8.15 Rule `parameter_9`

Rule `parameter_9` is an assignment rule for parameter `parameter_9`:

$$\text{parameter\_9} = \text{ModelValue\_6} - \frac{\text{species\_11}}{\text{vol}\left(\text{compartment\_2}\right)} \tag{35}$$

8.16 Rule `parameter_10`

Rule `parameter_10` is an assignment rule for parameter `parameter_10`:

$$\text{parameter\_10} = \text{ModelValue\_7} - \frac{\text{species\_13}}{\text{vol}\left(\text{compartment\_3}\right)} \tag{36}$$

8.17 Rule `parameter_20`

Rule `parameter_20` is an assignment rule for parameter `parameter_20`:

$$\text{parameter\_20} = \text{ModelValue\_16} - \frac{\text{species\_21}}{\text{vol}\left(\text{compartment\_2}\right)} \tag{37}$$

8.18 Rule `parameter_21`

Rule `parameter_21` is an assignment rule for parameter `parameter_21`:

$$\text{parameter\_21} = \text{ModelValue\_16} - \frac{\text{species\_22}}{\text{vol}\left(\text{compartment\_3}\right)} \tag{38}$$

8.19 Rule `F_in`

Rule `F_in` is an assignment rule for parameter `F_in`:

$$\text{F\_in} = \text{F\_0} \cdot \text{f\_CBF\_dyn} \tag{39}$$

8.20 Rule `F_out`

Rule `F_out` is an assignment rule for parameter `F_out`:

$$\text{F\_out} = \text{F\_0} \cdot \frac{\left(\frac{\text{vol(venous\_balloon)}}{\text{Compartment\_9}}\right)^{\frac{1}{0.5}} + \left(\frac{\text{vol(venous\_balloon)}}{\text{Compartment\_9}}\right)^{\frac{1}{2}} \cdot \frac{\text{tau\_v}}{\text{Compartment\_9}} \cdot \text{F\_in}}{1 + \text{F\_0} \cdot \left(\frac{\text{vol(venous\_balloon)}}{\text{Compartment\_9}}\right)^{\frac{1}{2}} \cdot \frac{\text{tau\_v}}{\text{Compartment\_9}}} \tag{40}$$

8.21 Rule `is_stimulated`

Rule `is_stimulated` is an assignment rule for parameter `is_stimulated`:

$$\text{is\_stimulated} = \begin{cases} 0 & \text{if } (\text{time} \leq 200) \vee (\text{time} \geq \text{t\_0} + \text{t\_end}) \\ 1 & \text{otherwise} \end{cases} \tag{41}$$

8.22 Rule `v_stim`

Rule `v_stim` is an assignment rule for parameter `v_stim`:

$$\text{v\_stim} = \text{is\_stimulated} \cdot \text{stimulus} \tag{42}$$

8.23 Rule `venous_balloon`

Rule `venous_balloon` is a rate rule for compartment `venous_balloon`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{vol}\left(\text{venous\_balloon}\right) = \text{F\_in} - \text{F\_out} \tag{43}$$

9 Reactions

This model contains 64 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	reaction_2	HK_astrocytes (R01786) (HeinrichSchuster)	species_5 + species_4 $\xrightarrow{\text{species\_6}}$ species_6 + ADP_astrocytes	0000176
2	reaction_5	PFK_neurons (R04779, R01070, R01015)	species_7 + species_3 ⟶ 2 species_9 + ADP_neurons	0000395
3	reaction_6	PFK_astrocytes (R04779, R01070, R01015)	species_8 + species_5 ⟶ 2 species_10 + ADP_astrocytes	0000395
4	reaction_7	PGK_neurons (R01061, R01512, R01518, R00658)	species_9 + ADP_neurons + NAD_neurons ⟶ species_11 + species_12 + species_3	0000395
5	reaction_8	PGK_astrocytes (R01061, R01512, R01518, R00658)	species_10 + ADP_astrocytes + NAD_astrocytes ⟶ species_13 + species_14 + species_5	0000395
6	reaction_9	PK_neurons (R00200)	species_12 + ADP_neurons ⟶ species_3 + species_15	0000176
7	reaction_10	PK_astrocytes (R00200)	species_14 + ADP_astrocytes ⟶ species_5 + species_17	0000176
8	reaction_13	mitochondrial_respiration_neurons (n.a.)	species_15 + 3 species_16 + species_11 + 15 ADP_neurons ⟶ 15 species_3 + 3 species_24 + NAD_neurons	0000395
9	reaction_14	mitochondrial_respiration_astrocytes (n.a.)	species_17 + 15 ADP_astrocytes + 3 species_20 + species_13 ⟶ 15 species_5 + 3 species_24 + NAD_astrocytes	0000395

№	Id	Name	Reaction Equation	SBO
10	reaction_17	GLC_exchange_extracellular_space_neurons (Aubert)	species_27 ⟶ species_1	0000185
11	reaction_18	GLC_exchange_extracellular_space-_astrocytes (Aubert)	species_27 ⟶ species_4	0000185
12	reaction_19	GLC_exchange_capillary_ec (Aubert)	species_25 ⟶ species_27	0000185
13	reaction_20	GLC_exchange_capillary_astrocytes (Aubert)	species_25 ⟶ species_4	0000185
14	reaction_21	LAC_exchange_ec_capillary	species_28 ⟶ species_26	0000185
15	reaction_22	LAC_exchange_neurons_ec	species_28 ⟶ species_18	0000185
16	reaction_23	LAC_exchange_astrocytes_ec	species_19 ⟶ species_28	0000185
17	reaction_24	LAC_exchange_astrocytes_capillary	species_19 ⟶ species_26	0000185
18	O2_exchange-_capillary-_neurons	O2_exchange_capillary_neurons	species_23 ⟶ species_16	0000185
19	O2_exchange-_capillary-_astrocytes	O2_exchange_capillary_astrocytes	species_23 ⟶ species_20	0000185
20	Blood_flow-_contribution-_to_capillary-_O2	O2_exchange_artery_capillary	O2_artery ⟶ species_23	0000185
21	Blood_flow-_contribution-_to_capillary-_GLC	GLC_exchange_artery_capillary	GLC_artery ⟶ species_25	0000185
22	Blood_flow-_contribution-_to_capillary-_LAC	LAC_exchange_capillary_artery	species_26 ⟶ LAC_artery	0000185

№	Id	Name	Reaction Equation	SBO
23	Flow_of_CO2-_between-_capillary-_and_vessel_-_artery_	CO2_exchange_capillary_artery	species_24 ⟶ CO2_artery	0000185
24	vPUMP_neurons	Na+_exchange_neurons_extracellular_space (n.a.)	species_3 + 3 Na__neurons ⟶ ADP_neurons	0000185
25	vPUMP-_astrocytes	Na+_exchange_astrocytes_extracellular_space (n.a.)	species_5 + 3 Na__astrocytes ⟶ ADP_astrocytes	0000185
26	vLEAK_Na-_neurons	LEAK_Na_neurons (n.a.)	Na__extracellular_space ⟶ Na__neurons	0000185
27	vLEAK_Na-_astrocytes	LEAK_Na_astrocytes (n.a)	Na__extracellular_space ⟶ Na__astrocytes	0000185
28	vSTIM	Na+_exchange_extracellular_space_neurons (stimulation)	Na__extracellular_space ⟶ Na__neurons	0000185
29	vGLU_ne	GLU_exchange_neurons_extracellular_space	GLU_neurons ⟶ GLU_extracellular_space	0000185
30	vGLU_eg	GLU_exchange_extracellular_space-_astrocytes	GLU_extracellular_space ⟶ GLU_astrocytes + Na__astrocytes	0000185
31	vGLU_gn	GLU_exchange_astrocytes_neurons	GLU_astrocytes + species_5 ⟶ GLU_neurons + ADP_astrocytes	0000185
32	inflow_of_dHb	inflow of dHb	$\emptyset \xrightarrow{\text{O2\_artery, species\_23}} \text{dHb}$	0000631
33	outflow_of_dHb	outflow of dHb	dHb ⟶ ∅	0000631
34	ATPase_neurons	ATPase_neurons (n.a.)	species_3 ⟶ ADP_neurons	0000631
35	ATPase-_astrocytes	ATPase_astrocytes (n.a.)	species_5 ⟶ ADP_astrocytes	0000631
36	AK_neurons	AK_neurons (R00127)	2 ADP_neurons ⟷ species_3 + AMP_neurons	
37	AK_astrocytes	AK_astrocytes (R00127)	2 ADP_astrocytes ⟷ species_5 + AMP_astrocytes	

№	Id	Name	Reaction Equation	SBO
38	CK_astrocytes-_forward_-_R01881	CK_astrocytes (R01881)	ADP_astrocytes + species_22 $\rightleftharpoons$ species_5 + Cr_astrocytes	
39	CK_neurons-_forward_-_R01881	CK_neurons (R01881)	species_21 + ADP_neurons $\rightleftharpoons$ species_3 + Cr_neurons	
40	LDH_astrocytes-_forward_-_R00703	LDH_astrocytes (R00703)	species_17 + species_13 $\rightleftharpoons$ species_19 + NAD_astrocytes	0000176
41	LDH_neurons-_forward_-_R00703	LDH_neurons (R00703)	species_15 + species_11 $\rightleftharpoons$ species_18 + NAD_neurons	0000176
42	ZWF_astrocytes-__R02736	ZWF_astrocytes (R02736)	species_6 + NADP_astrocytes $\longrightarrow$ G6L_astrocytes + NADPH_astrocytes	0000176
43	ZWF_neurons_-_R02736	ZWF_neurons (R02736)	species_2 + NADP_neurons $\longrightarrow$ G6L_neurons + NADPH_neurons	0000176
44	SOL_neurons_-_R02035	SOL_neurons (R02035)	G6L_neurons $\longrightarrow$ P6G_neurons	0000176
45	SOL_astrocytes-__R02035	SOL_astrocytes (R02035)	G6L_astrocytes $\longrightarrow$ P6G_astrocytes	0000176
46	GND_neurons__-_R01528	GND_neurons (R01528)	P6G_neurons + NADP_neurons $\rightleftharpoons$ Ru5P_neurons + NADPH_neurons	0000176
47	GND_astrocytes-__R01528	GND_astrocytes (R01528)	P6G_astrocytes + NADP_astrocytes $\longrightarrow$ Ru5P_astrocytes + NADPH_astrocytes	0000176
48	RPE_neurons_-_R01529	RPE_neurons (R01529)	Ru5P_neurons $\rightleftharpoons$ X5P_neurons	0000176
49	RPE_astrocytes-__R01529	RPE_astrocytes (R01529)	Ru5P_astrocytes $\rightleftharpoons$ X5P_astrocytes	0000176

№	Id	Name	Reaction Equation	SBO
50	RKI_astrocytes__R01056	RKI_astrocytes (R01056)	Ru5P_astrocytes $\rightleftharpoons$ R5P_astrocytes	0000176
51	RKI_neurons__R01056	RKI_neurons (R01056)	Ru5P_neurons $\rightleftharpoons$ R5P_neurons	0000176
52	TKL_1_astrocytes__R01641	TKL-1_astrocytes (R01641)	X5P_astrocytes + R5P_astrocytes $\longrightarrow$ species_10 + S7P_astrocytes	0000176
53	TKL_1_neurons__R01641	TKL-1_neurons (R01641)	X5P_neurons + R5P_neurons $\longrightarrow$ species_9 + S7P_neurons	0000176
54	TAL_astrocytes__R01827	TAL_astrocytes (R01827)	species_10 + S7P_astrocytes $\rightleftharpoons$ species_8 + E4P_astrocytes	0000176
55	TAL_neurons__R01827	TAL_neurons (R01827)	species_9 + S7P_neurons $\rightleftharpoons$ species_7 + E4P_neurons	0000176
56	TKL_2_astrocytes__R01830	TKL-2_astrocytes (R01830)	species_8 + species_10 $\longrightarrow$ X5P_astrocytes + E4P_astrocytes	0000176
57	TKL_2_neurons__R01830	TKL-2_neurons (R01830)	species_7 + species_9 $\longrightarrow$ X5P_neurons + E4P_neurons	0000176
58	NADPH_oxidase_neurons__R07172	NADPH oxidase neurons (R07172)	NADPH_neurons $\longrightarrow$ NADP_neurons	0000631
59	NADPH_oxidase_astrocytes__R07172	NADPH oxidase astrocytes (R07172)	NADPH_astrocytes $\longrightarrow$ NADP_astrocytes	0000631
60	R5P_sink_astrocytes__n_a_	R5P sink_astrocytes (n.a.)	R5P_astrocytes $\longrightarrow \emptyset$	0000631
61	R5P_sink_neurons__n_a_	R5P sink_neurons (n.a.)	R5P_neurons $\longrightarrow \emptyset$	0000631

№	Id	Name	Reaction Equation	SBO
62	PGI_astrocytes-__R02740___HS	PGI_astrocytes (R02740) (HS)	species_6 $\rightleftharpoons$ species_8	
63	HK_neurons-__R01786__-_HeinrichSchuster	HK_neurons (R01786) (HeinrichSchuster)	species_3 + species_1 $\xrightarrow{\text{species\_2}}$ species_2 + ADP_neurons	0000176
64	PGI_neurons_-_R02740___HS	PGI_neurons (R02740) (HS)	species_2 $\rightleftharpoons$ species_7	

9.1 Reaction `reaction_2`

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

Name HK_astrocytes (R01786) (HeinrichSchuster)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{species\_5} + \text{species\_4} \xrightarrow{\text{species\_6}} \text{species\_6} + \text{ADP\_astrocytes} \tag{44}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
`species_5`	ATP	
`species_4`	GLC	

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
`species_6`	G6P	

Products

Table 8: Properties of each product.

Id	Name	SBO
`species_6`	G6P	
`ADP_astrocytes`	ADP	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} v_1 = {} & \text{vol}\left(\text{compartment\_3}\right) \\ & \cdot \text{vHK\_\_HS}\left(\text{k\_HK}, \frac{\text{species\_5}}{\text{vol}\left(\text{compartment\_3}\right)}, \frac{\text{species\_6}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{K\_I\_G6P}\right) \end{aligned} \tag{45}$$

$$\mathrm{vHK\_\_HS}\left(\mathrm{k\_HK}, \mathrm{ATP}, \mathrm{G6P}, \mathrm{K\_I\_G6P}\right) = \mathrm{k\_HK} \cdot \mathrm{ATP} \cdot \left(1 + \frac{\mathrm{G6P}}{\mathrm{K\_I\_G6P}}\right)^{1} \tag{46}$$

$$\mathrm{vHK\_\_HS}\left(\mathrm{k\_HK}, \mathrm{ATP}, \mathrm{G6P}, \mathrm{K\_I\_G6P}\right) = \mathrm{k\_HK} \cdot \mathrm{ATP} \cdot \left(1 + \frac{\mathrm{G6P}}{\mathrm{K\_I\_G6P}}\right)^{1} \tag{47}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_HK	k_HK		0.01		☑
K_I_G6P	K_I_G6P		0.02		☑

9.2 Reaction reaction_5

This is an irreversible reaction of two reactants forming two products.

Name PFK_neurons (R04779, R01070, R01015)

SBO:0000395 encapsulating process

Reaction equation

$$\mathrm{species\_7} + \mathrm{species\_3} \longrightarrow 2\,\mathrm{species\_9} + \mathrm{ADP\_neurons} \tag{48}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
species_7	F6P	
species_3	ATP	

Products

Table 11: Properties of each product.

Id	Name	SBO
species_9	GAP	
ADP_neurons	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{vPFK}\left(\mathrm{k\_PFK}, \frac{\mathrm{species\_3}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \mathrm{parameter\_5}, \mathrm{parameter\_6}, \frac{\mathrm{species\_7}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \mathrm{K\_m\_F6P}\right) \tag{49}$$

$$\begin{aligned} &\mathrm{vPFK}\left(\mathrm{k\_PFK}, \mathrm{ATP}, \mathrm{K\_I\_ATP}, \mathrm{nH}, \mathrm{F6P}, \mathrm{K\_m\_F6P}\right) \\ &= \mathrm{k\_PFK} \cdot \mathrm{ATP} \cdot \left(1 + \left(\frac{\mathrm{ATP}}{\mathrm{K\_I\_ATP}}\right)^{\mathrm{nH}}\right)^{1} \cdot \frac{\mathrm{F6P}}{\mathrm{F6P} + \mathrm{K\_m\_F6P}} \end{aligned} \tag{50}$$

$$\begin{aligned} &\mathrm{vPFK}\left(\mathrm{k\_PFK}, \mathrm{ATP}, \mathrm{K\_I\_ATP}, \mathrm{nH}, \mathrm{F6P}, \mathrm{K\_m\_F6P}\right) \\ &= \mathrm{k\_PFK} \cdot \mathrm{ATP} \cdot \left(1 + \left(\frac{\mathrm{ATP}}{\mathrm{K\_I\_ATP}}\right)^{\mathrm{nH}}\right)^{1} \cdot \frac{\mathrm{F6P}}{\mathrm{F6P} + \mathrm{K\_m\_F6P}} \end{aligned} \tag{51}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_PFK	k_PFK		0.44		☑
K_m_F6P	K_m_F6P		0.18		☑

9.3 Reaction reaction_6

This is an irreversible reaction of two reactants forming two products.

Name PFK_astrocytes (R04779, R01070, R01015)

SBO:0000395 encapsulating process

Reaction equation

$$\mathrm{species\_8} + \mathrm{species\_5} \longrightarrow 2\,\mathrm{species\_10} + \mathrm{ADP\_astrocytes} \tag{52}$$

Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
species_8	F6P	
species_5	ATP	

Products

Table 14: Properties of each product.

Id	Name	SBO
species_10	GAP	
ADP_astrocytes	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\left(\mathrm{compartment\_3}\right) \cdot \mathrm{vPFK}\left(\mathrm{k\_PFK}, \frac{\mathrm{species\_5}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \mathrm{parameter\_5}, \mathrm{parameter\_6}, \frac{\mathrm{species\_8}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \mathrm{K\_m\_F6P}\right) \tag{53}$$

$$\begin{aligned} &\mathrm{vPFK}\left(\mathrm{k\_PFK}, \mathrm{ATP}, \mathrm{K\_I\_ATP}, \mathrm{nH}, \mathrm{F6P}, \mathrm{K\_m\_F6P}\right) \\ &= \mathrm{k\_PFK} \cdot \mathrm{ATP} \cdot \left(1 + \left(\frac{\mathrm{ATP}}{\mathrm{K\_I\_ATP}}\right)^{\mathrm{nH}}\right)^{1} \cdot \frac{\mathrm{F6P}}{\mathrm{F6P} + \mathrm{K\_m\_F6P}} \end{aligned} \tag{54}$$

$$\begin{aligned} &\mathrm{vPFK}\left(\mathrm{k\_PFK}, \mathrm{ATP}, \mathrm{K\_I\_ATP}, \mathrm{nH}, \mathrm{F6P}, \mathrm{K\_m\_F6P}\right) \\ &= \mathrm{k\_PFK} \cdot \mathrm{ATP} \cdot \left(1 + \left(\frac{\mathrm{ATP}}{\mathrm{K\_I\_ATP}}\right)^{\mathrm{nH}}\right)^{1} \cdot \frac{\mathrm{F6P}}{\mathrm{F6P} + \mathrm{K\_m\_F6P}} \end{aligned} \tag{55}$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_PFK	k_PFK		0.20		☑
K_m_F6P	K_m_F6P		0.18		☑

9.4 Reaction `reaction_7`

This is an irreversible reaction of three reactants forming three products.

Name PGK_neurons (R01061, R01512, R01518, R00658)

SBO:0000395 encapsulating process

Reaction equation

$$\text{species\_9} + \text{ADP\_neurons} + \text{NAD\_neurons} \longrightarrow \text{species\_11} + \text{species\_12} + \text{species\_3} \tag{56}$$

Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
`species_9`	GAP	
`ADP_neurons`	ADP	
`NAD_neurons`	NAD	

Products

Table 17: Properties of each product.

Id	Name	SBO
`species_11`	NADH	
`species_12`	PEP	
`species_3`	ATP	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}\left(\text{compartment\_2}\right) \cdot \text{vPGK}\left(\text{k\_PGK}, \frac{\text{species\_9}}{\text{vol}\left(\text{compartment\_2}\right)}, \frac{\text{ADP\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)}, \frac{\text{NAD\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)}, \frac{\text{species\_11}}{\text{vol}\left(\text{compartment\_2}\right)}\right) \tag{57}$$

$$\text{vPGK}\left(\text{k\_PGK}, \text{GAP}, \text{ADP}, \text{NAD}, \text{NADH}\right) = \text{k\_PGK} \cdot \text{GAP} \cdot \text{ADP} \cdot \frac{\text{NAD}}{\text{NADH}} \tag{58}$$

$$\text{vPGK}\left(\text{k\_PGK}, \text{GAP}, \text{ADP}, \text{NAD}, \text{NADH}\right) = \text{k\_PGK} \cdot \text{GAP} \cdot \text{ADP} \cdot \frac{\text{NAD}}{\text{NADH}} \tag{59}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_PGK	k_PGK		10.0		☑

9.5 Reaction reaction_8

This is an irreversible reaction of three reactants forming three products.

Name PGK_astrocytes (R01061, R01512, R01518, R00658)

SBO:0000395 encapsulating process

Reaction equation

$$\text{species\_10} + \text{ADP\_astrocytes} + \text{NAD\_astrocytes} \longrightarrow \text{species\_13} + \text{species\_14} + \text{species\_5} \tag{60}$$

Reactants

Table 19: Properties of each reactant.

Id	Name	SBO
species_10	GAP	
ADP_astrocytes	ADP	
NAD_astrocytes	NAD	

Products

Table 20: Properties of each product.

Id	Name	SBO
species_13	NADH	
species_14	PEP	
species_5	ATP	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\left(\mathrm{compartment\_3}\right) \cdot \mathrm{vPGK}\left(\mathrm{k\_PGK}, \frac{\mathrm{species\_10}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{ADP\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{NAD\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{species\_13}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}\right) \tag{61}$$

$$\mathrm{vPGK}\left(\mathrm{k\_PGK}, \mathrm{GAP}, \mathrm{ADP}, \mathrm{NAD}, \mathrm{NADH}\right) = \mathrm{k\_PGK} \cdot \mathrm{GAP} \cdot \mathrm{ADP} \cdot \frac{\mathrm{NAD}}{\mathrm{NADH}} \tag{62}$$

$$\mathrm{vPGK}\left(\mathrm{k\_PGK}, \mathrm{GAP}, \mathrm{ADP}, \mathrm{NAD}, \mathrm{NADH}\right) = \mathrm{k\_PGK} \cdot \mathrm{GAP} \cdot \mathrm{ADP} \cdot \frac{\mathrm{NAD}}{\mathrm{NADH}} \tag{63}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_PGK	k_PGK		3.0		☑

9.6 Reaction reaction_9

This is an irreversible reaction of two reactants forming two products.

Name PK_neurons (R00200)

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{species\_12} + \mathrm{ADP\_neurons} \longrightarrow \mathrm{species\_3} + \mathrm{species\_15} \tag{64}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
species_12	PEP	
ADP_neurons	ADP	

Products

Table 23: Properties of each product.

Id	Name	SBO
species_3	ATP	
species_15	PYR	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{vPK}\left(\mathrm{k\_PK}, \frac{\mathrm{species\_12}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{ADP\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}\right) \tag{65}$$

$$\mathrm{vPK}\left(\mathrm{k\_PK}, \mathrm{PEP}, \mathrm{ADP}\right) = \mathrm{k\_PK} \cdot \mathrm{PEP} \cdot \mathrm{ADP} \tag{66}$$

$$\mathrm{vPK}\left(\mathrm{k\_PK}, \mathrm{PEP}, \mathrm{ADP}\right) = \mathrm{k\_PK} \cdot \mathrm{PEP} \cdot \mathrm{ADP} \tag{67}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_PK	k_PK		44.0		☑

9.7 Reaction reaction_10

This is an irreversible reaction of two reactants forming two products.

Name PK_astrocytes (R00200)

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{species\_14} + \mathrm{ADP\_astrocytes} \longrightarrow \mathrm{species\_5} + \mathrm{species\_17} \tag{68}$$

Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
species_14	PEP	
ADP_astrocytes	ADP	

Products

Table 26: Properties of each product.

Id	Name	SBO
species_5	ATP	
species_17	PYR	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\left(\mathrm{compartment\_3}\right) \cdot \mathrm{vPK}\left(\mathrm{k\_PK}, \frac{\mathrm{species\_14}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{ADP\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}\right) \tag{69}$$

$$\mathrm{vPK}\left(\mathrm{k\_PK}, \mathrm{PEP}, \mathrm{ADP}\right) = \mathrm{k\_PK} \cdot \mathrm{PEP} \cdot \mathrm{ADP} \tag{70}$$

$$\mathrm{vPK}\left(\mathrm{k\_PK}, \mathrm{PEP}, \mathrm{ADP}\right) = \mathrm{k\_PK} \cdot \mathrm{PEP} \cdot \mathrm{ADP} \tag{71}$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_PK	k_PK		20.0		☑

9.8 Reaction reaction_13

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

Name mitochondrial_respiration_neurons (n.a.)

SBO:0000395 encapsulating process

Reaction equation

$$\mathrm{species\_15} + 3\,\mathrm{species\_16} + \mathrm{species\_11} + 15\,\mathrm{ADP\_neurons} \longrightarrow 15\,\mathrm{species\_3} + 3\,\mathrm{species\_24} + \mathrm{NAD\_neurons} \tag{72}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
species_15	PYR	
species_16	O2	
species_11	NADH	
ADP_neurons	ADP	

Products

Table 29: Properties of each product.

Id	Name	SBO
species_3	ATP	
species_24	CO2	
NAD_neurons	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vMITO2\_\_inkl\_\_Volumes}\left(\text{v\_max\_mito}, \frac{\text{species\_15}}{\text{vol}\left(\text{compartment\_2}\right)}, \text{parameter\_18}, \frac{\text{ADP\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)}, \text{parameter\_16}, \frac{\text{species\_16}}{\text{vol}\left(\text{compartment\_2}\right)}, \text{parameter\_17}, \text{alpha}, \frac{\text{species\_3}}{\text{vol}\left(\text{compartment\_2}\right)}, \text{beta}, \text{vol}\left(\text{compartment\_2}\right)\right) \tag{73}$$

$$\text{vMITO2\_\_inkl\_\_Volumes}\left(\text{v\_max\_mito}, \text{PYR}, \text{K\_m\_PYR}, \text{ADP}, \text{K\_m\_ADP}, \text{O2}, \text{K\_m\_O2}, \text{alpha}, \text{ATP}, \text{beta}, \text{Volume}\right) = \text{v\_max\_mito} \cdot \frac{\text{PYR}}{\text{PYR} + \text{K\_m\_PYR}} \cdot \frac{\text{ADP}}{\text{ADP} + \text{K\_m\_ADP}} \cdot \frac{\text{O2}}{\text{O2} + \text{K\_m\_O2}} \cdot \left(1 - \frac{1}{1 + \exp\left(\text{alpha} \cdot \left(\frac{\text{ATP}}{\text{ADP}} - \text{beta}\right)\right)}\right) \cdot \text{Volume} \tag{74}$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v_max_mito	v_max_mito		0.1		☑
alpha	alpha		5.0		☑
beta	beta		20.0		☑

9.9 Reaction reaction_14

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

Name mitochondrial_respiration_astrocytes (n.a.)

SBO:0000395 encapsulating process

Reaction equation

$$\text{species\_17} + 15\,\text{ADP\_astrocytes} + 3\,\text{species\_20} + \text{species\_13} \longrightarrow 15\,\text{species\_5} + 3\,\text{species\_24} + \text{NAD\_astrocytes} \tag{75}$$

Reactants

Table 31: Properties of each reactant.

Id	Name	SBO
species_17	PYR	
ADP_astrocytes	ADP	
species_20	O2	
species_13	NADH	

Products

Table 32: Properties of each product.

Id	Name	SBO
species_5	ATP	
species_24	CO2	
NAD_astrocytes	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vMITO2\_\_inkl\_\_Volumes}\left(\text{v\_max\_mito}, \frac{\text{species\_17}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{parameter\_18}, \frac{\text{ADP\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{parameter\_16}, \frac{\text{species\_20}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{parameter\_17}, \text{alpha}, \frac{\text{species\_5}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{beta}, \text{vol}\left(\text{compartment\_3}\right)\right) \tag{76}$$

$$\begin{aligned}\text{vMITO2\_\_inkl\_\_Volumes}\left(\text{v\_max\_mito}, \text{PYR}, \text{K\_m\_PYR}, \text{ADP}, \text{K\_m\_ADP}, \text{O2}, \text{K\_m\_O2},\right.\\ \left.\text{alpha}, \text{ATP}, \text{beta}, \text{Volume}\right) = \text{v\_max\_mito} \cdot \frac{\text{PYR}}{\text{PYR} + \text{K\_m\_PYR}} \cdot \frac{\text{ADP}}{\text{ADP} + \text{K\_m\_ADP}}\\ \cdot \frac{\text{O2}}{\text{O2} + \text{K\_m\_O2}} \cdot \left(1 - \frac{1}{1 + \exp\left(\text{alpha} \cdot \left(\frac{\text{ATP}}{\text{ADP}} - \text{beta}\right)\right)}\right) \cdot \text{Volume}\end{aligned} \tag{77}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v_max_mito	v_max_mito		0.01		☑
alpha	alpha		5.00		☑
beta	beta		20.00		☑

9.10 Reaction reaction_17

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

Name GLC_exchange_extracellular_space_neurons (Aubert)

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_27} \longrightarrow \text{species\_1} \tag{78}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
species_27	GLC	

Product

Table 35: Properties of each product.

Id	Name	SBO
species_1	GLC	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{facilitated\_transport\_\_inkl\_\_Volume\_\_\_\_scaled}\left(\text{Vmax\_en\_GLC\_\_wrt\_neurons\_\_\_Aubert}, \text{\_sf}, \frac{\text{species\_27}}{\text{vol}\left(\text{compartment\_4}\right)}, \text{K\_T\_GLC\_en\_\_Aubert}, \frac{\text{species\_1}}{\text{vol}\left(\text{compartment\_2}\right)}, \text{vol}\left(\text{compartment\_4}\right)\right) \tag{79}$$

$$\begin{aligned} &\text{facilitated\_transport\_\_inkl\_\_Volume\_\_\_\_scaled}\left(\text{Vmax}, \text{sf}, \text{S}, \text{K}, \text{P}, \text{Volume}\right) \\ &= \text{Vmax} \cdot \text{sf} \cdot \left(\frac{\text{S}}{\text{S}+\text{K}} - \frac{\text{P}}{\text{P}+\text{K}}\right) \cdot \text{Volume} \end{aligned} \tag{80}$$

9.11 Reaction `reaction_18`

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

Name GLC_exchange_extracellular_space_astrocytes (Aubert)

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_27} \longrightarrow \text{species\_4} \tag{81}$$

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
`species_27`	GLC	

Product

Table 37: Properties of each product.

Id	Name	SBO
`species_4`	GLC	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{facilitated\_transport\_\_inkl\_\_Volume\_\_\_\_scaled}\left(\text{Vmax\_eg\_GLC\_\_wrt\_astrocytes\_\_\_Aubert\_}, \text{\_sf}, \frac{\text{species\_27}}{\text{vol}\left(\text{compartment\_4}\right)}, \text{K\_T\_GLC\_eg\_\_Aubert}, \frac{\text{species\_4}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{vol}\left(\text{compartment\_4}\right)\right) \tag{82}$$

$$\begin{aligned} &\text{facilitated\_transport\_\_inkl\_\_Volume\_\_\_\_scaled}\left(\text{Vmax}, \text{sf}, \text{S}, \text{K}, \text{P}, \text{Volume}\right) \\ &= \text{Vmax} \cdot \text{sf} \cdot \left(\frac{\text{S}}{\text{S}+\text{K}} - \frac{\text{P}}{\text{P}+\text{K}}\right) \cdot \text{Volume} \end{aligned} \tag{83}$$

9.12 Reaction `reaction_19`

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

Name GLC_exchange_capillary_ec (Aubert)

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_25} \longrightarrow \text{species\_27} \tag{84}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
`species_25`	GLC	

Product

Table 39: Properties of each product.

Id	Name	SBO
`species_27`	GLC	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{facilitated\_transport\_\_inkl\_\_Volume\_\_\_\_scaled}\left(\text{Vmax\_ce\_GLC\_\_wrt\_capillaries\_\_\_Aubert}, \text{\_sf}, \frac{\text{species\_25}}{\text{vol}\left(\text{compartment\_1}\right)}, \text{K\_T\_GLC\_ce\_\_Aubert}, \frac{\text{species\_27}}{\text{vol}\left(\text{compartment\_4}\right)}, \text{vol}\left(\text{compartment\_1}\right)\right) \tag{85}$$

$$\begin{aligned} &\text{facilitated\_transport\_\_inkl\_\_Volume\_\_\_\_scaled}\left(\text{Vmax}, \text{sf}, \text{S}, \text{K}, \text{P}, \text{Volume}\right) \\ &= \text{Vmax} \cdot \text{sf} \cdot \left(\frac{\text{S}}{\text{S}+\text{K}} - \frac{\text{P}}{\text{P}+\text{K}}\right) \cdot \text{Volume} \end{aligned} \tag{86}$$

9.13 Reaction `reaction_20`

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

Name GLC_exchange_capillary_astrocytes (Aubert)

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_25} \longrightarrow \text{species\_4} \tag{87}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
`species_25`	GLC	

Product

Table 41: Properties of each product.

Id	Name	SBO
`species_4`	GLC	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{facilitated\_transport\_\_inkl\_\_Volume\_\_\_\_scaled}\left(\text{Vmax\_cg\_GLC\_\_wrt\_capillaries\_\_\_Aubert}, \text{\_sf}, \frac{\text{species\_25}}{\text{vol}\left(\text{compartment\_1}\right)}, \text{K\_T\_GLC\_cg\_\_Aubert}, \frac{\text{species\_4}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{vol}\left(\text{compartment\_1}\right)\right) \tag{88}$$

$$\begin{aligned} &\text{facilitated\_transport\_\_inkl\_\_Volume\_\_\_\_scaled}\left(\text{Vmax}, \text{sf}, \text{S}, \text{K}, \text{P}, \text{Volume}\right) \\ &= \text{Vmax} \cdot \text{sf} \cdot \left(\frac{\text{S}}{\text{S}+\text{K}} - \frac{\text{P}}{\text{P}+\text{K}}\right) \cdot \text{Volume} \end{aligned} \tag{89}$$

9.14 Reaction `reaction_21`

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

Name LAC_exchange_ec_capillary

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_28} \longrightarrow \text{species\_26} \tag{90}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
`species_28`	LAC	

Product

Table 43: Properties of each product.

Id	Name	SBO
`species_26`	LAC	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{facilitated\_transport\_\_inkl\_\_Volume}\left(\text{Vmax\_ec\_LAC\_\_wrt\_extracellular\_space\_\_\_Aubert}, \frac{\text{species\_28}}{\text{vol}\left(\text{compartment\_4}\right)}, \text{K\_T\_LAC\_ec\_\_Aubert}, \frac{\text{species\_26}}{\text{vol}\left(\text{compartment\_1}\right)}, \text{vol}\left(\text{compartment\_4}\right)\right) \tag{91}$$

$$\begin{aligned} &\text{facilitated\_transport\_\_inkl\_\_Volume}\left(\text{Vmax}, \text{S}, \text{K}, \text{P}, \text{Volume}\right) \\ &= \text{Vmax} \cdot \left(\frac{\text{S}}{\text{S} + \text{K}} - \frac{\text{P}}{\text{P} + \text{K}}\right) \cdot \text{Volume} \end{aligned} \tag{92}$$

9.15 Reaction `reaction_22`

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

Name LAC_exchange_neurons_ec

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_28} \longrightarrow \text{species\_18} \tag{93}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
`species_28`	LAC	

Product

Table 45: Properties of each product.

Id	Name	SBO
`species_18`	LAC	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{facilitated\_transport\_\_inkl\_\_Volume}\left(\text{Vmax\_ne\_LAC\_\_wrt\_neurons\_\_\_Aubert}, \frac{\text{species\_28}}{\text{vol}\left(\text{compartment\_4}\right)}, \text{K\_T\_LAC\_ne\_\_Aubert}, \frac{\text{species\_18}}{\text{vol}\left(\text{compartment\_2}\right)}, \text{vol}\left(\text{compartment\_4}\right)\right) \tag{94}$$

$$\begin{aligned} &\text{facilitated\_transport\_\_inkl\_\_Volume}\left(\text{Vmax}, \text{S}, \text{K}, \text{P}, \text{Volume}\right) \\ &= \text{Vmax} \cdot \left(\frac{\text{S}}{\text{S} + \text{K}} - \frac{\text{P}}{\text{P} + \text{K}}\right) \cdot \text{Volume} \end{aligned} \tag{95}$$

9.16 Reaction `reaction_23`

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

Name LAC_exchange_astrocytes_ec

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_19} \longrightarrow \text{species\_28} \tag{96}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
`species_19`	LAC	

Product

Table 47: Properties of each product.

Id	Name	SBO
`species_28`	LAC	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{facilitated\_transport\_\_inkl\_\_Volume}\left(\text{Vmax\_ge\_LAC\_\_wrt\_astrocytes\_\_\_Aubert}, \frac{\text{species\_19}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{K\_T\_LAC\_ge\_\_Aubert}, \frac{\text{species\_28}}{\text{vol}\left(\text{compartment\_4}\right)}, \text{vol}\left(\text{compartment\_3}\right)\right) \tag{97}$$

$$\begin{aligned} &\text{facilitated\_transport\_\_inkl\_\_Volume}\left(\text{Vmax}, \text{S}, \text{K}, \text{P}, \text{Volume}\right) \\ &= \text{Vmax} \cdot \left(\frac{\text{S}}{\text{S} + \text{K}} - \frac{\text{P}}{\text{P} + \text{K}}\right) \cdot \text{Volume} \end{aligned} \tag{98}$$

9.17 Reaction `reaction_24`

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

Name LAC_exchange_astrocytes_capillary

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_19} \longrightarrow \text{species\_26} \tag{99}$$

Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
`species_19`	LAC	

Product

Table 49: Properties of each product.

Id	Name	SBO
`species_26`	LAC	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{facilitated\_transport\_\_inkl\_\_Volume}\left(\text{Vmax\_gc\_LAC\_\_wrt\_astrocytes\_\_\_Aubert}, \frac{\text{species\_19}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{K\_T\_LAC\_gc\_\_Aubert}, \frac{\text{species\_26}}{\text{vol}\left(\text{compartment\_1}\right)}, \text{vol}\left(\text{compartment\_3}\right)\right) \tag{100}$$

$$\begin{aligned} &\text{facilitated\_transport\_\_inkl\_\_Volume}\left(\text{Vmax}, \text{S}, \text{K}, \text{P}, \text{Volume}\right) \\ &= \text{Vmax} \cdot \left(\frac{\text{S}}{\text{S} + \text{K}} - \frac{\text{P}}{\text{P} + \text{K}}\right) \cdot \text{Volume} \end{aligned} \tag{101}$$

9.18 Reaction `O2_exchange_capillary_neurons`

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

Name O2_exchange_capillary_neurons

SBO:0000185 transport reaction

Notes `O2 exchange between capillary and neurons`

Reaction equation

$$\text{species\_23} \longrightarrow \text{species\_16} \tag{102}$$

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
`species_23`	O2	

Product

Table 51: Properties of each product.

Id	Name	SBO
`species_16`	O2	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{O2\_transport\_function\_inkl\_\_volume}\left(\text{PS\_cap\_neuron\_\_wrt\_capillaries\_\_\_Aubert},\right.$$
$$\text{vol}\left(\text{compartment\_2}\right), \text{K\_O2\_\_Aubert}, \text{Hb\_OP}, \frac{\text{species\_23}}{\text{vol}\left(\text{compartment\_1}\right)}, \text{nh\_O2\_\_Aubert},$$
$$\left.\frac{\text{species\_16}}{\text{vol}\left(\text{compartment\_2}\right)}, \text{vol}\left(\text{compartment\_1}\right)\right) \tag{103}$$

$$\begin{aligned}\text{O2\_transport\_function\_inkl\_\_volume}\left(\text{PScap}, \text{Volume}, \text{KO2},\right.&\\ \left.\text{HbOP}, \text{O2\_source}, \text{nh}, \text{O2\_destination}, \text{Volume1}\right) &= \frac{\text{PScap}}{\text{Volume}}\\ \cdot \left(\text{KO2} \cdot \left(\frac{\text{HbOP}}{\text{O2\_source}} - 1\right)^{\frac{1}{\text{nh}}} - \text{O2\_destination}\right) &\cdot \text{Volume1}\end{aligned} \tag{104}$$

9.19 Reaction `O2_exchange_capillary_astrocytes`

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

Name O2_exchange_capillary_astrocytes

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_23} \longrightarrow \text{species\_20} \tag{105}$$

Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
`species_23`	O2	

Product

Table 53: Properties of each product.

Id	Name	SBO
species_20	O2	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{O2\_transport\_function\_inkl\_\_volume}\left(\text{PScap}, \text{vol}\left(\text{compartment\_3}\right), \text{K\_O2\_\_Aubert}, \text{Hb\_OP}, \frac{\text{species\_23}}{\text{vol}\left(\text{compartment\_1}\right)}, \text{nh\_O2\_\_Aubert}, \frac{\text{species\_20}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{vol}\left(\text{compartment\_1}\right)\right) \tag{106}$$

$$\begin{aligned}\text{O2\_transport\_function\_inkl\_\_volume}\left(\text{PScap}, \text{Volume}, \text{KO2}, \text{HbOP}, \text{O2\_source}, \text{nh}, \text{O2\_destination}, \text{Volume1}\right) &= \frac{\text{PScap}}{\text{Volume}} \\ \cdot \left(\text{KO2} \cdot \left(\frac{\text{HbOP}}{\text{O2\_source}} - 1\right)^{\frac{1}{\text{nh}}} - \text{O2\_destination}\right) &\cdot \text{Volume1}\end{aligned} \tag{107}$$

Table 54: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PScap	PScap		10.0		☑

9.20 Reaction Blood_flow_contribution_to_capillary_O2

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

Name O2_exchange_artery_capillary

SBO:0000185 transport reaction

Reaction equation

$$\text{O2\_artery} \longrightarrow \text{species\_23} \tag{108}$$

Reactant

Table 55: Properties of each reactant.

Id	Name	SBO
O2_artery	O2	

Product

Table 56: Properties of each product.

Id	Name	SBO
species_23	O2	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{Blood\_flow\_contribution\_inkl\_volume}\left(\text{F\_in}, \text{vol}\left(\text{compartment\_1}\right), \text{vol}\left(\text{artery}\right), \frac{\text{O2\_artery}}{\text{vol}\left(\text{artery}\right)}, \frac{\text{species\_23}}{\text{vol}\left(\text{compartment\_1}\right)}\right) \tag{109}$$

$$\begin{aligned}&\text{Blood\_flow\_contribution\_inkl\_volume}\left(\text{F\_in}, \text{V\_c}, \text{Volume}, \text{Substrate}, \text{Product}\right)\\ &= \frac{2 \cdot \text{F\_in}}{\text{V\_c}} \cdot \left(\text{Substrate} - \text{Product}\right) \cdot \text{Volume}\end{aligned} \tag{110}$$

9.21 Reaction Blood_flow_contribution_to_capillary_GLC

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

Name GLC_exchange_artery_capillary

SBO:0000185 transport reaction

Reaction equation

$$\text{GLC\_artery} \longrightarrow \text{species\_25} \tag{111}$$

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
GLC_artery	GLC	

Product

Table 58: Properties of each product.

Id	Name	SBO
species_25	GLC	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{Blood\_flow\_contribution\_inkl\_volume}\left(\text{F\_in}, \text{vol}\left(\text{compartment\_1}\right), \text{vol}\left(\text{artery}\right), \frac{\text{GLC\_artery}}{\text{vol}\left(\text{artery}\right)}, \frac{\text{species\_25}}{\text{vol}\left(\text{compartment\_1}\right)}\right) \tag{112}$$

$$\begin{aligned}&\text{Blood\_flow\_contribution\_inkl\_volume}\left(\text{F\_in}, \text{V\_c}, \text{Volume}, \text{Substrate}, \text{Product}\right)\\ &= \frac{2 \cdot \text{F\_in}}{\text{V\_c}} \cdot \left(\text{Substrate} - \text{Product}\right) \cdot \text{Volume}\end{aligned} \tag{113}$$

9.22 Reaction Blood_flow_contribution_to_capillary_LAC

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

Name LAC_exchange_capillary_artery

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_26} \longrightarrow \text{LAC\_artery} \tag{114}$$

Reactant

Table 59: Properties of each reactant.

Id	Name	SBO
species_26	LAC	

Product

Table 60: Properties of each product.

Id	Name	SBO
LAC_artery	LAC	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{Blood\_flow\_contribution\_inkl\_\_volume}\left(\text{F\_in}, \text{vol}\left(\text{compartment\_1}\right), \text{vol}\left(\text{compartment\_1}\right), \frac{\text{species\_26}}{\text{vol}\left(\text{compartment\_1}\right)}, \frac{\text{LAC\_artery}}{\text{vol}\left(\text{artery}\right)}\right) \tag{115}$$

$$\text{Blood\_flow\_contribution\_inkl\_\_volume}\left(\text{F\_in}, \text{V\_c}, \text{Volume}, \text{Substrate}, \text{Product}\right) = \frac{2 \cdot \text{F\_in}}{\text{V\_c}} \cdot \left(\text{Substrate} - \text{Product}\right) \cdot \text{Volume} \tag{116}$$

9.23 Reaction Flow_of_CO2_between_capillary_and_vessel__artery_

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

Name CO2_exchange_capillary_artery

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_24} \longrightarrow \text{CO2\_artery} \tag{117}$$

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
species_24	CO2	

Product

Table 62: Properties of each product.

Id	Name	SBO
CO2_artery	CO2	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{Blood\_flow\_contribution\_inkl\_\_volume}\left(\text{F\_in}, \text{vol}\left(\text{compartment\_1}\right), \text{vol}\left(\text{compartment\_1}\right), \frac{\text{species\_24}}{\text{vol}\left(\text{compartment\_1}\right)}, \frac{\text{CO2\_artery}}{\text{vol}\left(\text{artery}\right)}\right) \tag{118}$$

$$\begin{aligned}&\text{Blood\_flow\_contribution\_inkl\_\_volume}\left(\text{F\_in}, \text{V\_c}, \text{Volume}, \text{Substrate}, \text{Product}\right)\\ &= \frac{2 \cdot \text{F\_in}}{\text{V\_c}} \cdot \left(\text{Substrate} - \text{Product}\right) \cdot \text{Volume}\end{aligned} \tag{119}$$

9.24 Reaction vPUMP_neurons

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

Name Na+_exchange_neurons_extracellular_space (n.a.)

SBO:0000185 transport reaction

Reaction equation

$$\text{species\_3} + 3\,\text{Na\_\_neurons} \longrightarrow \text{ADP\_neurons} \tag{120}$$

Reactants

Table 63: Properties of each reactant.

Id	Name	SBO
species_3	ATP	
Na__neurons	Na+	

Product

Table 64: Properties of each product.

Id	Name	SBO
ADP_neurons	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{vPUMP\_volume\_dependent}\left(\mathrm{Sm\_n}, \mathrm{vol}\left(\mathrm{compartment\_2}\right), \mathrm{k\_pump}, \frac{\mathrm{species\_3}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{Na\_\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \mathrm{K\_m\_Na\_pump}\right) \tag{121}$$

$$\begin{aligned}&\mathrm{vPUMP\_volume\_dependent}\left(\mathrm{Sm}, \mathrm{Volume}, \mathrm{k\_pump}, \mathrm{ATP}, \mathrm{Na}, \mathrm{Km\_pump}\right)\\ &= \frac{\mathrm{Sm}}{\mathrm{Volume}} \cdot \mathrm{k\_pump} \cdot \mathrm{ATP} \cdot \mathrm{Na} \cdot \left(1 + \frac{\mathrm{ATP}}{\mathrm{Km\_pump}}\right)^{1}\end{aligned} \tag{122}$$

$$\begin{aligned}&\mathrm{vPUMP\_volume\_dependent}\left(\mathrm{Sm}, \mathrm{Volume}, \mathrm{k\_pump}, \mathrm{ATP}, \mathrm{Na}, \mathrm{Km\_pump}\right)\\ &= \frac{\mathrm{Sm}}{\mathrm{Volume}} \cdot \mathrm{k\_pump} \cdot \mathrm{ATP} \cdot \mathrm{Na} \cdot \left(1 + \frac{\mathrm{ATP}}{\mathrm{Km\_pump}}\right)^{1}\end{aligned} \tag{123}$$

9.25 Reaction vPUMP_astrocytes

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

Name Na+_exchange_astrocytes_extracellular_space (n.a.)

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{species\_5} + 3\,\mathrm{Na\_\_astrocytes} \longrightarrow \mathrm{ADP\_astrocytes} \tag{124}$$

Reactants

Table 65: Properties of each reactant.

Id	Name	SBO
species_5	ATP	
Na__astrocytes	Na+	

Product

Table 66: Properties of each product.

Id	Name	SBO
ADP_astrocytes	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \mathrm{vol}\left(\mathrm{compartment\_3}\right) \cdot \mathrm{vPUMP\_volume\_dependent}\left(\mathrm{Sm\_g}, \mathrm{vol}\left(\mathrm{compartment\_3}\right), \mathrm{k\_pump}, \frac{\mathrm{species\_5}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{Na\_\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \mathrm{K\_m\_Na\_pump}\right) \tag{125}$$

$$\begin{aligned}&\mathrm{vPUMP\_volume\_dependent}\left(\mathrm{Sm}, \mathrm{Volume}, \mathrm{k\_pump}, \mathrm{ATP}, \mathrm{Na}, \mathrm{Km\_pump}\right)\\ &= \frac{\mathrm{Sm}}{\mathrm{Volume}} \cdot \mathrm{k\_pump} \cdot \mathrm{ATP} \cdot \mathrm{Na} \cdot \left(1 + \frac{\mathrm{ATP}}{\mathrm{Km\_pump}}\right)^{1}\end{aligned} \tag{126}$$

$$\begin{aligned}&\mathrm{vPUMP\_volume\_dependent}\left(\mathrm{Sm}, \mathrm{Volume}, \mathrm{k\_pump}, \mathrm{ATP}, \mathrm{Na}, \mathrm{Km\_pump}\right)\\ &= \frac{\mathrm{Sm}}{\mathrm{Volume}} \cdot \mathrm{k\_pump} \cdot \mathrm{ATP} \cdot \mathrm{Na} \cdot \left(1 + \frac{\mathrm{ATP}}{\mathrm{Km\_pump}}\right)^{1}\end{aligned} \tag{127}$$

9.26 Reaction vLEAK_Na_neurons

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

Name LEAK_Na_neurons (n.a.)

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{Na\_\_extracellular\_space} \longrightarrow \mathrm{Na\_\_neurons} \tag{128}$$

Reactant

Table 67: Properties of each reactant.

Id	Name	SBO
Na__extracellular_space	Na+	

Product

Table 68: Properties of each product.

Id	Name	SBO
Na__neurons	Na+	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \text{vLEAK\_Na\_inkl\_\_Volume}\left(\text{Sm\_n}, \text{g\_Na\_neurons}, \text{vol}\left(\text{compartment\_2}\right), \text{F}, \text{RT}, \frac{\text{Na\_\_extracellular\_space}}{\text{vol}\left(\text{compartment\_4}\right)}, \frac{\text{Na\_\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)}, \text{Vm}, \text{vol}\left(\text{compartment\_2}\right)\right) \tag{129}$$

$$\text{vLEAK\_Na\_inkl\_\_Volume}\left(\text{Sm}, \text{gNA}, \text{Volume}, \text{F}, \text{RT}, \text{Na\_e}, \text{Na}, \text{Vm}, \text{Volume1}\right) = \frac{\text{Sm} \cdot \text{gNA}}{\text{Volume} \cdot \text{F}} \cdot \left(\frac{\text{RT}}{\text{F}} \cdot \left(\frac{\text{Na\_e}}{\text{Na}}\right) - \text{Vm}\right) \cdot \text{Volume1} \tag{130}$$

9.27 Reaction vLEAK_Na_astrocytes

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

Name LEAK_Na_astrocytes (n.a)

SBO:0000185 transport reaction

Reaction equation

$$\text{Na\_\_extracellular\_space} \longrightarrow \text{Na\_\_astrocytes} \tag{131}$$

Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
Na__extracellular_space	Na+	

Product

Table 70: Properties of each product.

Id	Name	SBO
Na__astrocytes	Na+	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \text{vLEAK\_Na\_inkl\_\_Volume}\left(\text{Sm\_g}, \text{gNA}, \text{vol}\left(\text{compartment\_3}\right), \text{F}, \text{RT}, \frac{\text{Na\_\_extracellular\_space}}{\text{vol}\left(\text{compartment\_4}\right)}, \frac{\text{Na\_\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{Vm}, \text{vol}\left(\text{compartment\_3}\right)\right) \tag{132}$$

$$\text{vLEAK\_Na\_inkl\_\_Volume}\left(\text{Sm}, \text{gNA}, \text{Volume}, \text{F}, \text{RT}, \text{Na\_e}, \text{Na}, \text{Vm}, \text{Volume1}\right) = \frac{\text{Sm} \cdot \text{gNA}}{\text{Volume} \cdot \text{F}} \cdot \left(\frac{\text{RT}}{\text{F}} \cdot \left(\frac{\text{Na\_e}}{\text{Na}}\right) - \text{Vm}\right) \cdot \text{Volume1} \tag{133}$$

Table 71: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
gNA	gNA		0.004		☑

9.28 Reaction vSTIM

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

Name Na+_exchange_extracellular_space_neurons (stimulation)

SBO:0000185 transport reaction

Reaction equation

$$\text{Na\_\_extracellular\_space} \longrightarrow \text{Na\_\_neurons} \tag{134}$$

Reactant

Table 72: Properties of each reactant.

Id	Name	SBO
Na__extracellular_space	Na+	

Product

Table 73: Properties of each product.

Id	Name	SBO
Na__neurons	Na+	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \text{vStim\_\_with\_volume}\left(\text{v\_stim}, \text{vol}\left(\text{compartment\_2}\right)\right) \tag{135}$$

$$\text{vStim\_\_with\_volume}\left(\text{vstim}, \text{Volume}\right) = \text{vstim} \cdot \text{Volume} \tag{136}$$

9.29 Reaction vGLU_ne

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

Name GLU_exchange_neurons_extracellular_space

SBO:0000185 transport reaction

Notes Glutamate release by neurons to extracellular space

Reaction equation

$$\text{GLU\_neurons} \longrightarrow \text{GLU\_extracellular\_space} \tag{137}$$

Reactant

Table 74: Properties of each reactant.

Id	Name	SBO
GLU_neurons	GLU	

Product

Table 75: Properties of each product.

Id	Name	SBO
GLU_extracellular_space	GLU	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \text{vGLU\_ne\_\_inkl\_\_Volume}\left(\text{v\_stim}, \text{R\_Na\_GLU}, \frac{\text{GLU\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)}, \text{K\_m\_GLU}, \text{vol}\left(\text{compartment\_2}\right)\right) \tag{138}$$

$$\begin{aligned} &\text{vGLU\_ne\_\_inkl\_\_Volume}\left(\text{vSTIM}, \text{ratio\_Na\_GLU}, \text{GLU\_n}, \text{Km\_GLU}, \text{Volume}\right) \\ &= \text{vSTIM} \cdot \text{ratio\_Na\_GLU} \cdot \frac{\text{GLU\_n}}{\text{GLU\_n} + \text{Km\_GLU}} \cdot \text{Volume} \end{aligned} \tag{139}$$

9.30 Reaction vGLU_eg

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

Name GLU_exchange_extracellular_space_astrocytes

SBO:0000185 transport reaction

Reaction equation

$$\text{GLU\_extracellular\_space} \longrightarrow \text{GLU\_astrocytes} + \text{Na\_\_astrocytes} \tag{140}$$

Reactant

Table 76: Properties of each reactant.

Id	Name	SBO
GLU_extracellular_space	GLU	

Products

Table 77: Properties of each product.

Id	Name	SBO
GLU_astrocytes	GLU	
Na__astrocytes	Na+	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \text{vGLU\_eg\_\_inkl\_\_Volumes}\left(\text{Vmax\_eg\_GLU\_\_wrt\_extracellular\_space}, \frac{\text{GLU\_extracellular\_space}}{\text{vol}\left(\text{compartment\_4}\right)}, \text{K\_m\_GLU}, \text{vol}\left(\text{compartment\_4}\right)\right) \tag{141}$$

$$\begin{aligned} &\text{vGLU\_eg\_\_inkl\_\_Volumes}\left(\text{Vmax\_GLU}, \text{GLU\_e}, \text{K\_m\_GLU}, \text{Volume}\right) \\ &= \text{Vmax\_GLU} \cdot \frac{\text{GLU\_e}}{\text{GLU\_e} + \text{K\_m\_GLU}} \cdot \text{Volume} \end{aligned} \tag{142}$$

9.31 Reaction vGLU_gn

This is an irreversible reaction of two reactants forming two products.

Name GLU_exchange_astrocytes_neurons

SBO:0000185 transport reaction

Reaction equation

$$\text{GLU\_astrocytes} + \text{species\_5} \longrightarrow \text{GLU\_neurons} + \text{ADP\_astrocytes} \tag{143}$$

Reactants

Table 78: Properties of each reactant.

Id	Name	SBO
GLU_astrocytes	GLU	
species_5	ATP	

Products

Table 79: Properties of each product.

Id	Name	SBO
GLU_neurons	GLU	
ADP_astrocytes	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \text{vGLU\_gn\_\_inkl\_\_Volume}\left(\text{V\_gn\_max\_GLU}, \frac{\text{GLU\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{K\_m\_GLU}, \frac{\text{species\_5}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{parameter\_14}, \text{vol}\left(\text{compartment\_3}\right)\right) \tag{144}$$

$$\begin{aligned}&\text{vGLU\_gn\_\_inkl\_\_Volume}\left(\text{Vmax\_GLU}, \text{GLU\_g}, \text{K\_m\_GLU}, \text{ATP\_g}, \text{K\_m\_ATP}, \text{Volume}\right)\\ &= \text{Vmax\_GLU} \cdot \frac{\text{GLU\_g}}{\text{GLU\_g} + \text{K\_m\_GLU}} \cdot \frac{\text{ATP\_g}}{\text{ATP\_g} + \text{K\_m\_ATP}} \cdot \text{Volume}\end{aligned} \tag{145}$$

9.32 Reaction inflow_of_dHb

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

Name inflow of dHb

SBO:0000631 pseudoreaction

Reaction equation

$$\emptyset \xrightarrow{\text{O2\_artery, species\_23}} \text{dHb} \tag{146}$$

Modifiers

Table 80: Properties of each modifier.

Id	Name	SBO
O2_artery	O2	
species_23	O2	

Product

Table 81: Properties of each product.

Id	Name	SBO
dHb	dHb	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{vdHb\_in}\left(\mathrm{F\_in}, \frac{\mathrm{O2\_artery}}{\mathrm{vol}\left(\mathrm{artery}\right)}, \frac{\mathrm{species\_23}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}\right) \tag{147}$$

$$\mathrm{vdHb\_in}\left(\mathrm{F\_in}, \mathrm{O2\_a}, \mathrm{O2\_c}\right) = \mathrm{F\_in} \cdot \left(\mathrm{O2\_a} - 2 \cdot \mathrm{O2\_c} - \mathrm{O2\_a}\right) \tag{148}$$

$$\mathrm{vdHb\_in}\left(\mathrm{F\_in}, \mathrm{O2\_a}, \mathrm{O2\_c}\right) = \mathrm{F\_in} \cdot \left(\mathrm{O2\_a} - 2 \cdot \mathrm{O2\_c} - \mathrm{O2\_a}\right) \tag{149}$$

9.33 Reaction outflow_of_dHb

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

Name outflow of dHb

SBO:0000631 pseudoreaction

Reaction equation

$$\mathrm{dHb} \longrightarrow \emptyset \tag{150}$$

Reactant

Table 82: Properties of each reactant.

Id	Name	SBO
dHb	dHb	

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{vdHb\_out}\left(\mathrm{F\_out}, \frac{\mathrm{dHb}}{\mathrm{vol}\left(\mathrm{compartment\_1}\right)}, \mathrm{vol}\left(\mathrm{venous\_balloon}\right)\right) \tag{151}$$

$$\mathrm{vdHb\_out}\left(\mathrm{F\_out}, \mathrm{dHb}, \mathrm{V\_v}\right) = \frac{\mathrm{F\_out} \cdot \mathrm{dHb}}{\mathrm{V\_v}} \tag{152}$$

$$\mathrm{vdHb\_out}\left(\mathrm{F\_out}, \mathrm{dHb}, \mathrm{V\_v}\right) = \frac{\mathrm{F\_out} \cdot \mathrm{dHb}}{\mathrm{V\_v}} \tag{153}$$

9.34 Reaction `ATPase_neurons`

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

Name ATPase_neurons (n.a.)

SBO:0000631 pseudoreaction

Reaction equation

$$\mathrm{species\_3} \longrightarrow \mathrm{ADP\_neurons} \tag{154}$$

Reactant

Table 83: Properties of each reactant.

Id	Name	SBO
`species_3`	ATP	

Product

Table 84: Properties of each product.

Id	Name	SBO
`ADP_neurons`	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{vATPase}\left(\mathrm{VmaxATPase}, \frac{\mathrm{species\_3}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \mathrm{K\_m\_ATP\_ATPase}\right) \tag{155}$$

$$\mathrm{vATPase}\left(\mathrm{VmaxATPase}, \mathrm{ATP}, \mathrm{Km\_ATP}\right) = \mathrm{VmaxATPase} \cdot \frac{\mathrm{ATP}}{\mathrm{ATP} + \mathrm{Km\_ATP}} \tag{156}$$

$$\mathrm{vATPase}\left(\mathrm{VmaxATPase}, \mathrm{ATP}, \mathrm{Km\_ATP}\right) = \mathrm{VmaxATPase} \cdot \frac{\mathrm{ATP}}{\mathrm{ATP} + \mathrm{Km\_ATP}} \qquad (157)$$

Table 85: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmaxATPase	VmaxATPase		0.07		☑

9.35 Reaction ATPase_astrocytes

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

Name ATPase_astrocytes (n.a.)

SBO:0000631 pseudoreaction

Reaction equation

$$\text{species\_5} \longrightarrow \text{ADP\_astrocytes} \tag{158}$$

Reactant

Table 86: Properties of each reactant.

Id	Name	SBO
species_5	ATP	

Product

Table 87: Properties of each product.

Id	Name	SBO
ADP_astrocytes	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \text{vol}\left(\text{compartment\_3}\right) \cdot \text{vATPase}\left(\text{VmaxATPase}, \frac{\text{species\_5}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{K\_m\_ATP\_ATPase}\right) \tag{159}$$

$$\text{vATPase}\left(\text{VmaxATPase}, \text{ATP}, \text{Km\_ATP}\right) = \text{VmaxATPase} \cdot \frac{\text{ATP}}{\text{ATP} + \text{Km\_ATP}} \tag{160}$$

$$\mathrm{vATPase}\left(\mathrm{VmaxATPase}, \mathrm{ATP}, \mathrm{Km\_ATP}\right) = \mathrm{VmaxATPase} \cdot \frac{\mathrm{ATP}}{\mathrm{ATP} + \mathrm{Km\_ATP}} \qquad (161)$$

Table 88: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmaxATPase	VmaxATPase		0.035		☑

9.36 Reaction AK_neurons

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

Name AK_neurons (R00127)

Reaction equation

$$2\,\mathrm{ADP\_neurons} \rightleftharpoons \mathrm{species\_3} + \mathrm{AMP\_neurons} \tag{162}$$

Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
ADP_neurons	ADP	

Products

Table 90: Properties of each product.

Id	Name	SBO
species_3	ATP	
AMP_neurons	AMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \left(\mathrm{k1} \cdot \left(\frac{\mathrm{ADP\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)} \right)^2 - \mathrm{k2} \cdot \frac{\mathrm{species\_3}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)} \cdot \frac{\mathrm{AMP\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)} \right) \tag{163}$$

Table 91: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		1000.0		☑
k2	k2		920.0		☑

9.37 Reaction AK_astrocytes

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

Name AK_astrocytes (R00127)

Reaction equation

$$2\,\text{ADP\_astrocytes} \rightleftharpoons \text{species\_5} + \text{AMP\_astrocytes} \tag{164}$$

Reactant

Table 92: Properties of each reactant.

Id	Name	SBO
ADP_astrocytes	ADP	

Products

Table 93: Properties of each product.

Id	Name	SBO
species_5	ATP	
AMP_astrocytes	AMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{37} = \text{vol}\left(\text{compartment\_3}\right) \cdot \left(\text{k1} \cdot \left(\frac{\text{ADP\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)} \right)^2 - \text{k2} \cdot \frac{\text{species\_5}}{\text{vol}\left(\text{compartment\_3}\right)} \cdot \frac{\text{AMP\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)} \right) \tag{165}$$

Table 94: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		1000.0		☑
k2	k2		920.0		☑

9.38 Reaction CK_astrocytes_forward__R01881

This is a reversible reaction of two reactants forming two products.

Name CK_astrocytes (R01881)

Reaction equation

$$\text{ADP\_astrocytes} + \text{species\_22} \rightleftharpoons \text{species\_5} + \text{Cr\_astrocytes} \tag{166}$$

Reactants

Table 95: Properties of each reactant.

Id	Name	SBO
ADP_astrocytes	ADP	
species_22	PCr	

Products

Table 96: Properties of each product.

Id	Name	SBO
species_5	ATP	
Cr_astrocytes	Cr	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \text{vol}\left(\text{compartment\_3}\right) \cdot \left(\text{k1} \cdot \frac{\text{ADP\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)} \cdot \frac{\text{species\_22}}{\text{vol}\left(\text{compartment\_3}\right)} - \text{k2} \cdot \frac{\text{species\_5}}{\text{vol}\left(\text{compartment\_3}\right)} \cdot \frac{\text{Cr\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)} \right) \tag{167}$$

Table 97: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.50		☑
k2	k2		0.01		☑

9.39 Reaction CK_neurons_forward__R01881

This is a reversible reaction of two reactants forming two products.

Name CK_neurons (R01881)

Reaction equation

$$\text{species\_21} + \text{ADP\_neurons} \rightleftharpoons \text{species\_3} + \text{Cr\_neurons} \tag{168}$$

Reactants

Table 98: Properties of each reactant.

Id	Name	SBO
species_21	PCr	
ADP_neurons	ADP	

Products

Table 99: Properties of each product.

Id	Name	SBO
species_3	ATP	
Cr_neurons	Cr	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = \text{vol}\left(\text{compartment\_2}\right) \cdot \left(\text{k1} \cdot \frac{\text{species\_21}}{\text{vol}\left(\text{compartment\_2}\right)} \cdot \frac{\text{ADP\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)} - \text{k2} \cdot \frac{\text{species\_3}}{\text{vol}\left(\text{compartment\_2}\right)} \cdot \frac{\text{Cr\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)} \right) \tag{169}$$

Table 100: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.50		☑
k2	k2		0.01		☑

9.40 Reaction LDH_astrocytes_forward__R00703

This is a reversible reaction of two reactants forming two products.

Name LDH_astrocytes (R00703)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{species\_17} + \text{species\_13} \rightleftharpoons \text{species\_19} + \text{NAD\_astrocytes} \tag{170}$$

Reactants

Table 101: Properties of each reactant.

Id	Name	SBO
species_17	PYR	
species_13	NADH	

Products

Table 102: Properties of each product.

Id	Name	SBO
species_19	LAC	
NAD_astrocytes	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{40} = \text{vol}\left(\text{compartment\_3}\right) \cdot \left(\text{k1} \cdot \frac{\text{species\_17}}{\text{vol}\left(\text{compartment\_3}\right)} \cdot \frac{\text{species\_13}}{\text{vol}\left(\text{compartment\_3}\right)} - \text{k2} \cdot \frac{\text{species\_19}}{\text{vol}\left(\text{compartment\_3}\right)} \cdot \frac{\text{NAD\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)} \right) \tag{171}$$

Table 103: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		780.0		☑
k2	k2		32.0		☑

9.41 Reaction LDH_neurons_forward_R00703

This is a reversible reaction of two reactants forming two products.

Name LDH_neurons (R00703)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{species\_15} + \text{species\_11} \rightleftharpoons \text{species\_18} + \text{NAD\_neurons} \tag{172}$$

Reactants

Table 104: Properties of each reactant.

Id	Name	SBO
species_15	PYR	
species_11	NADH	

Products

Table 105: Properties of each product.

Id	Name	SBO
species_18	LAC	
NAD_neurons	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = \text{vol}\left(\text{compartment\_2}\right) \cdot \left(\text{k1} \cdot \frac{\text{species\_15}}{\text{vol}\left(\text{compartment\_2}\right)} \cdot \frac{\text{species\_11}}{\text{vol}\left(\text{compartment\_2}\right)} - \text{k2} \cdot \frac{\text{species\_18}}{\text{vol}\left(\text{compartment\_2}\right)} \cdot \frac{\text{NAD\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)} \right) \tag{173}$$

Table 106: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		2000.0		☑
k2	k2		15.0		☑

9.42 Reaction ZWF_astrocytes__R02736

This is an irreversible reaction of two reactants forming two products.

Name ZWF_astrocytes (R02736)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{species\_6} + \text{NADP\_astrocytes} \longrightarrow \text{G6L\_astrocytes} + \text{NADPH\_astrocytes} \quad (174)$$

Reactants

Table 107: Properties of each reactant.

Id	Name	SBO
species_6	G6P	
NADP_astrocytes	NADP	

Products

Table 108: Properties of each product.

Id	Name	SBO
G6L_astrocytes	G6L	
NADPH_astrocytes	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = \text{vol}\left(\text{compartment\_3}\right) \cdot \text{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\text{Vmax}, \text{K\_S1}, \text{K\_S2}, \frac{\text{species\_6}}{\text{vol}\left(\text{compartment\_3}\right)}, \frac{\text{NADP\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)}, \frac{\text{G6L\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)}, \frac{\text{NADPH\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{Keq}, \text{K\_P1}, \text{K\_P2}\right) \tag{175}$$

$$\begin{aligned}\text{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\text{Vmax}, \text{K\_S1}, \text{K\_S2}, \text{S1}, \text{S2}, \text{P1}, \text{P2}, \text{Keq}, \text{K\_P1}, \text{K\_P2}\right) &= \text{Vmax} \cdot \frac{1}{\text{K\_S1} \cdot \text{K\_S2}} \\ \cdot \frac{\text{S1} \cdot \text{S2} - \frac{\text{P1} \cdot \text{P2}}{\text{Keq}}}{\left(1 + \frac{\text{S1}}{\text{K\_S1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{K\_S2}}\right) + \left(1 + \frac{\text{P1}}{\text{K\_P1}}\right) \cdot \left(1 + \frac{\text{P2}}{\text{K\_P2}}\right) - 1}&\end{aligned} \tag{176}$$

$$\begin{aligned}\text{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\text{Vmax}, \text{K\_S1}, \text{K\_S2}, \text{S1}, \text{S2}, \text{P1}, \text{P2}, \text{Keq}, \text{K\_P1}, \text{K\_P2}\right) &= \text{Vmax} \cdot \frac{1}{\text{K\_S1} \cdot \text{K\_S2}} \\ \cdot \frac{\text{S1} \cdot \text{S2} - \frac{\text{P1} \cdot \text{P2}}{\text{Keq}}}{\left(1 + \frac{\text{S1}}{\text{K\_S1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{K\_S2}}\right) + \left(1 + \frac{\text{P1}}{\text{K\_P1}}\right) \cdot \left(1 + \frac{\text{P2}}{\text{K\_P2}}\right) - 1}&\end{aligned} \tag{177}$$

Table 109: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		0.291		☑
K_S1	K_S1		$6.91392 \cdot 10^{-5}$		☑
K_S2	K_S2		$1.31616 \cdot 10^{-5}$		☑
Keq	Keq		22906.400		☑
K_P1	K_P1		0.018		☑
K_P2	K_P2		$5.0314 \cdot 10^{-4}$		☑

9.43 Reaction ZWF_neurons__R02736

This is an irreversible reaction of two reactants forming two products.

Name ZWF_neurons (R02736)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{species\_2} + \text{NADP\_neurons} \longrightarrow \text{G6L\_neurons} + \text{NADPH\_neurons} \tag{178}$$

Reactants

Table 110: Properties of each reactant.

Id	Name	SBO
species_2	G6P	
NADP_neurons	NADP	

Products

Table 111: Properties of each product.

Id	Name	SBO
G6L_neurons	G6L	
NADPH_neurons	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{43} = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \frac{\mathrm{species\_2}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{NADP\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{G6L\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{NADPH\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) \tag{179}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{180}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{181}$$

Table 112: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		0.586		☑
K_S1	K_S1		$6.91392 \cdot 10^{-5}$		☑
K_S2	K_S2		$1.31616 \cdot 10^{-5}$		☑
Keq	Keq		22906.400		☑
K_P1	K_P1		0.018		☑
K_P2	K_P2		$5.0314 \cdot 10^{-4}$		☑

9.44 Reaction SOL_neurons__R02035

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

Name SOL_neurons (R02035)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{G6L\_neurons} \longrightarrow \text{P6G\_neurons} \tag{182}$$

Reactant

Table 113: Properties of each reactant.

Id	Name	SBO
G6L_neurons	G6L	

Product

Table 114: Properties of each product.

Id	Name	SBO
P6G_neurons	P6G	

Kinetic Law

Derived unit contains undeclared units

$$v_{44} = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \frac{\mathrm{G6L\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{P6G\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \mathrm{Keq}, \mathrm{K\_P1}\right) \tag{183}$$

$$\begin{aligned}&\mathrm{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{S1}, \mathrm{P1}, \mathrm{Keq}, \mathrm{K\_P1}\right)\\ &= \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1}} \cdot \frac{\mathrm{S1} - \frac{\mathrm{P1}}{\mathrm{Keq}}}{1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}} + 1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}} - 1}\end{aligned} \tag{184}$$

$$\begin{aligned}&\mathrm{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{S1}, \mathrm{P1}, \mathrm{Keq}, \mathrm{K\_P1}\right)\\ &= \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1}} \cdot \frac{\mathrm{S1} - \frac{\mathrm{P1}}{\mathrm{Keq}}}{1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}} + 1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}} - 1}\end{aligned} \tag{185}$$

Table 115: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		0.373		☑
K_S1	K_S1		0.018		☑
Keq	Keq		531174.000		☑
K_P1	K_P1		2.286		☑

9.45 Reaction SOL_astrocytes__R02035

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

Name SOL_astrocytes (R02035)

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{G6L\_astrocytes} \longrightarrow \mathrm{P6G\_astrocytes} \tag{186}$$

Reactant

Table 116: Properties of each reactant.

Id	Name	SBO
G6L_astrocytes	G6L	

Product

Table 117: Properties of each product.

Id	Name	SBO
P6G_astrocytes	P6G	

Kinetic Law

Derived unit contains undeclared units

$$v_{45} = \mathrm{vol}\left(\mathrm{compartment\_3}\right) \cdot \mathrm{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \frac{\mathrm{G6L\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{P6G\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \mathrm{Keq}, \mathrm{K\_P1}\right) \tag{187}$$

$$\begin{aligned}&\mathrm{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{S1}, \mathrm{P1}, \mathrm{Keq}, \mathrm{K\_P1}\right)\\ &= \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1}} \cdot \frac{\mathrm{S1} - \frac{\mathrm{P1}}{\mathrm{Keq}}}{1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}} + 1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}} - 1}\end{aligned} \tag{188}$$

$$\begin{aligned}&\mathrm{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{S1}, \mathrm{P1}, \mathrm{Keq}, \mathrm{K\_P1}\right)\\ &= \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1}} \cdot \frac{\mathrm{S1} - \frac{\mathrm{P1}}{\mathrm{Keq}}}{1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}} + 1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}} - 1}\end{aligned} \tag{189}$$

Table 118: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		0.185		☑
K_S1	K_S1		0.018		☑
Keq	Keq		531174.000		☑
K_P1	K_P1		2.286		☑

9.46 Reaction GND_neurons___R01528

This is a reversible reaction of two reactants forming two products.

Name GND_neurons (R01528)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{P6G\_neurons} + \text{NADP\_neurons} \rightleftharpoons \text{Ru5P\_neurons} + \text{NADPH\_neurons} \tag{190}$$

Reactants

Table 119: Properties of each reactant.

Id	Name	SBO
P6G_neurons	P6G	
NADP_neurons	NADP	

Products

Table 120: Properties of each product.

Id	Name	SBO
Ru5P_neurons	Ru5P	
NADPH_neurons	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{46} = \text{vol}(\text{compartment\_2}) \cdot \text{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\text{Vmax}, \text{K\_S1}, \text{K\_S2}, \frac{\text{P6G\_neurons}}{\text{vol}(\text{compartment\_2})}, \frac{\text{NADP\_neurons}}{\text{vol}(\text{compartment\_2})}, \frac{\text{Ru5P\_neurons}}{\text{vol}(\text{compartment\_2})}, \frac{\text{NADPH\_neurons}}{\text{vol}(\text{compartment\_2})}, \text{Keq}, \text{K\_P1}, \text{K\_P2}\right) \tag{191}$$

$$\text{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}(\text{Vmax}, \text{K\_S1}, \text{K\_S2}, \text{S1}, \text{S2}, \text{P1}, \text{P2}, \text{Keq}, \text{K\_P1}, \text{K\_P2}) = \text{Vmax} \cdot \frac{1}{\text{K\_S1} \cdot \text{K\_S2}} \cdot \frac{\text{S1} \cdot \text{S2} - \frac{\text{P1} \cdot \text{P2}}{\text{Keq}}}{\left(1 + \frac{\text{S1}}{\text{K\_S1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{K\_S2}}\right) + \left(1 + \frac{\text{P1}}{\text{K\_P1}}\right) \cdot \left(1 + \frac{\text{P2}}{\text{K\_P2}}\right) - 1} \tag{192}$$

$$\begin{aligned}&\text{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\text{Vmax}, \text{K\_S1},\right.\\&\left.\text{K\_S2}, \text{S1}, \text{S2}, \text{P1}, \text{P2}, \text{Keq}, \text{K\_P1}, \text{K\_P2}\right) = \text{Vmax} \cdot \frac{1}{\text{K\_S1} \cdot \text{K\_S2}}\\&\cdot \frac{\text{S1} \cdot \text{S2} - \frac{\text{P1} \cdot \text{P2}}{\text{Keq}}}{\left(1 + \frac{\text{S1}}{\text{K\_S1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{K\_S2}}\right) + \left(1 + \frac{\text{P1}}{\text{K\_P1}}\right) \cdot \left(1 + \frac{\text{P2}}{\text{K\_P2}}\right) - 1}\end{aligned} \tag{193}$$

Table 121: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		2.658		☑
K_S1	K_S1		$3.23421 \cdot 10^{-5}$		☑
K_S2	K_S2		$3.11043 \cdot 10^{-6}$		☑
Keq	Keq		$4.0852 \cdot 10^{7}$		☑
K_P1	K_P1		0.054		☑
K_P2	K_P2		$5.0314 \cdot 10^{-4}$		☑

9.47 Reaction GND_astrocytes__R01528

This is an irreversible reaction of two reactants forming two products.

Name GND_astrocytes (R01528)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{P6G\_astrocytes} + \text{NADP\_astrocytes} \longrightarrow \text{Ru5P\_astrocytes} + \text{NADPH\_astrocytes} \tag{194}$$

Reactants

Table 122: Properties of each reactant.

Id	Name	SBO
P6G_astrocytes	P6G	
NADP_astrocytes	NADP	

Products

Table 123: Properties of each product.

Id	Name	SBO
Ru5P_astrocytes	Ru5P	
NADPH_astrocytes	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{47} = \mathrm{vol}\left(\mathrm{compartment\_3}\right) \cdot \mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \frac{\mathrm{P6G\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{NADP\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{Ru5P\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{NADPH\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) \tag{195}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{196}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{197}$$

Table 124: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		1.317		☑
K_S1	K_S1		$3.23421 \cdot 10^{-5}$		☑
K_S2	K_S2		$3.11043 \cdot 10^{-6}$		☑
Keq	Keq		$4.0852 \cdot 10^{7}$		☑
K_P1	K_P1		$5.0314 \cdot 10^{-4}$		☑
K_P2	K_P2		0.054		☑

9.48 Reaction RPE_neurons__R01529

This is a reversible reaction of one reactant forming one product.

Name RPE_neurons (R01529)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{Ru5P\_neurons} \rightleftharpoons \text{X5P\_neurons} \tag{198}$$

Reactant

Table 125: Properties of each reactant.

Id	Name	SBO
Ru5P_neurons	Ru5P	

Product

Table 126: Properties of each product.

Id	Name	SBO
X5P_neurons	X5P	

Kinetic Law

Derived unit contains undeclared units

$$v_{48} = \text{vol}\left(\text{compartment\_2}\right) \cdot \text{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\text{Vmax}, \text{K\_S1}, \frac{\text{Ru5P\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)}, \frac{\text{X5P\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)}, \text{Keq}, \text{K\_P1}\right) \tag{199}$$

$$\text{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\text{Vmax}, \text{K\_S1}, \text{S1}, \text{P1}, \text{Keq}, \text{K\_P1}\right) = \text{Vmax} \cdot \frac{1}{\text{K\_S1}} \cdot \frac{\text{S1} - \frac{\text{P1}}{\text{Keq}}}{1 + \frac{\text{S1}}{\text{K\_S1}} + 1 + \frac{\text{P1}}{\text{K\_P1}} - 1} \tag{200}$$

$$\text{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\text{Vmax}, \text{K\_S1}, \text{S1}, \text{P1}, \text{Keq}, \text{K\_P1}\right) = \text{Vmax} \cdot \frac{1}{\text{K\_S1}} \cdot \frac{\text{S1} - \frac{\text{P1}}{\text{Keq}}}{1 + \frac{\text{S1}}{\text{K\_S1}} + 1 + \frac{\text{P1}}{\text{K\_P1}} - 1} \tag{201}$$

Table 127: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		0.016		☑
K_S1	K_S1		0.054		☑
Keq	Keq		39.257		☑
K_P1	K_P1		0.603		☑

9.49 Reaction RPE_astrocytes__R01529

This is a reversible reaction of one reactant forming one product.

Name RPE_astrocytes (R01529)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{Ru5P\_astrocytes} \rightleftharpoons \text{X5P\_astrocytes} \tag{202}$$

Reactant

Table 128: Properties of each reactant.

Id	Name	SBO
Ru5P_astrocytes	Ru5P	

Product

Table 129: Properties of each product.

Id	Name	SBO
X5P_astrocytes	X5P	

Kinetic Law

Derived unit contains undeclared units

$$v_{49} = \text{vol}\left(\text{compartment\_3}\right) \cdot \text{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\text{Vmax}, \text{K\_S1}, \frac{\text{Ru5P\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)}, \frac{\text{X5P\_astrocytes}}{\text{vol}\left(\text{compartment\_3}\right)}, \text{Keq}, \text{K\_P1}\right) \tag{203}$$

$$\text{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}(\text{Vmax}, \text{K\_S1}, \text{S1}, \text{P1}, \text{Keq}, \text{K\_P1}) = \text{Vmax} \cdot \frac{1}{\text{K\_S1}} \cdot \frac{\text{S1} - \frac{\text{P1}}{\text{Keq}}}{1 + \frac{\text{S1}}{\text{K\_S1}} + 1 + \frac{\text{P1}}{\text{K\_P1}} - 1} \tag{204}$$

$$\text{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}(\text{Vmax}, \text{K\_S1}, \text{S1}, \text{P1}, \text{Keq}, \text{K\_P1}) = \text{Vmax} \cdot \frac{1}{\text{K\_S1}} \cdot \frac{\text{S1} - \frac{\text{P1}}{\text{Keq}}}{1 + \frac{\text{S1}}{\text{K\_S1}} + 1 + \frac{\text{P1}}{\text{K\_P1}} - 1} \tag{205}$$

Table 130: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		0.008		☑
K_S1	K_S1		0.054		☑
Keq	Keq		39.257		☑
K_P1	K_P1		0.603		☑

9.50 Reaction RKI_astrocytes__R01056

This is a reversible reaction of one reactant forming one product.

Name RKI_astrocytes (R01056)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{Ru5P\_astrocytes} \rightleftharpoons \text{R5P\_astrocytes} \tag{206}$$

Reactant

Table 131: Properties of each reactant.

Id	Name	SBO
Ru5P_astrocytes	Ru5P	

Product

Table 132: Properties of each product.

Id	Name	SBO
R5P_astrocytes	R5P	

Kinetic Law

Derived unit contains undeclared units

$$v_{50} = \mathrm{vol}\left(\mathrm{compartment\_3}\right) \cdot \mathrm{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \frac{\mathrm{Ru5P\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{R5P\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \mathrm{Keq}, \mathrm{K\_P1}\right) \tag{207}$$

$$\begin{aligned}&\mathrm{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{S1}, \mathrm{P1}, \mathrm{Keq}, \mathrm{K\_P1}\right)\\ &= \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1}} \cdot \frac{\mathrm{S1} - \frac{\mathrm{P1}}{\mathrm{Keq}}}{1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}} + 1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}} - 1}\end{aligned} \tag{208}$$

$$\begin{aligned}&\mathrm{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{S1}, \mathrm{P1}, \mathrm{Keq}, \mathrm{K\_P1}\right)\\ &= \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1}} \cdot \frac{\mathrm{S1} - \frac{\mathrm{P1}}{\mathrm{Keq}}}{1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}} + 1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}} - 1}\end{aligned} \tag{209}$$

Table 133: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		$8.21984 \cdot 10^{-4}$		☑
K_S1	K_S1		0.054		☑
Keq	Keq		35.453		☑
K_P1	K_P1		0.778		☑

9.51 Reaction RKI_neurons__R01056

This is a reversible reaction of one reactant forming one product.

Name RKI_neurons (R01056)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{Ru5P\_neurons} \rightleftharpoons \text{R5P\_neurons} \tag{210}$$

Reactant

Table 134: Properties of each reactant.

Id	Name	SBO
Ru5P_neurons	Ru5P	

Product

Table 135: Properties of each product.

Id	Name	SBO
R5P_neurons	R5P	

Kinetic Law

Derived unit contains undeclared units

$$v_{51} = \text{vol}\left(\text{compartment\_2}\right) \cdot \text{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\text{Vmax}, \text{K\_S1}, \frac{\text{Ru5P\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)}, \frac{\text{R5P\_neurons}}{\text{vol}\left(\text{compartment\_2}\right)}, \text{Keq}, \text{K\_P1}\right) \tag{211}$$

$$\begin{aligned}&\text{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\text{Vmax}, \text{K\_S1}, \text{S1}, \text{P1}, \text{Keq}, \text{K\_P1}\right)\\ &= \text{Vmax} \cdot \frac{1}{\text{K\_S1}} \cdot \frac{\text{S1} - \frac{\text{P1}}{\text{Keq}}}{1 + \frac{\text{S1}}{\text{K\_S1}} + 1 + \frac{\text{P1}}{\text{K\_P1}} - 1}\end{aligned} \tag{212}$$

$$\begin{aligned}&\text{modular\_rate\_law\_for\_one\_substrate\_\_one\_product}\left(\text{Vmax}, \text{K\_S1}, \text{S1}, \text{P1}, \text{Keq}, \text{K\_P1}\right)\\ &= \text{Vmax} \cdot \frac{1}{\text{K\_S1}} \cdot \frac{\text{S1} - \frac{\text{P1}}{\text{Keq}}}{1 + \frac{\text{S1}}{\text{K\_S1}} + 1 + \frac{\text{P1}}{\text{K\_P1}} - 1}\end{aligned} \tag{213}$$

Table 136: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		0.002		☑
K_S1	K_S1		0.054		☑
Keq	Keq		35.453		☑
K_P1	K_P1		0.778		☑

9.52 Reaction TKL_1_astrocytes__R01641

This is an irreversible reaction of two reactants forming two products.

Name TKL-1_astrocytes (R01641)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{X5P\_astrocytes} + \text{R5P\_astrocytes} \longrightarrow \text{species\_10} + \text{S7P\_astrocytes} \tag{214}$$

Reactants

Table 137: Properties of each reactant.

Id	Name	SBO
X5P_astrocytes	X5P	
R5P_astrocytes	R5P	

Products

Table 138: Properties of each product.

Id	Name	SBO
species_10	GAP	
S7P_astrocytes	S7P	

Kinetic Law

Derived unit contains undeclared units

$$v_{52} = \mathrm{vol}\left(\mathrm{compartment\_3}\right) \cdot \mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \frac{\mathrm{X5P\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{R5P\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{species\_10}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{S7P\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) \tag{215}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{216}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{217}$$

Table 139: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		$2.44278 \cdot 10^{-4}$		☑
K_S1	K_S1		$1.73625 \cdot 10^{-4}$		☑
K_S2	K_S2		$5.85387 \cdot 10^{-4}$		☑
Keq	Keq		1652870.000		☑
K_P1	K_P1		0.168		☑
K_P2	K_P2		0.193		☑

9.53 Reaction TKL_1_neurons__R01641

This is an irreversible reaction of two reactants forming two products.

Name TKL-1_neurons (R01641)

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{X5P\_neurons} + \mathrm{R5P\_neurons} \longrightarrow \mathrm{species\_9} + \mathrm{S7P\_neurons} \tag{218}$$

Reactants

Table 140: Properties of each reactant.

Id	Name	SBO
X5P_neurons	X5P	
R5P_neurons	R5P	

Products

Table 141: Properties of each product.

Id	Name	SBO
species_9	GAP	
S7P_neurons	S7P	

Kinetic Law

Derived unit contains undeclared units

$$v_{53} = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \frac{\mathrm{X5P\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{R5P\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{species\_9}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{S7P\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) \tag{219}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{220}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{221}$$

Table 142: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		$4.93027 \cdot 10^{-4}$		☑
K_S1	K_S1		$1.73625 \cdot 10^{-4}$		☑
K_S2	K_S2		$5.85387 \cdot 10^{-4}$		☑
Keq	Keq		1652870.000		☑
K_P1	K_P1		0.168		☑
K_P2	K_P2		0.193		☑

9.54 Reaction TAL_astrocytes__R01827

This is a reversible reaction of two reactants forming two products.

Name TAL_astrocytes (R01827)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{species\_10} + \text{S7P\_astrocytes} \rightleftharpoons \text{species\_8} + \text{E4P\_astrocytes} \tag{222}$$

Reactants

Table 143: Properties of each reactant.

Id	Name	SBO
species_10	GAP	
S7P_astrocytes	S7P	

Products

Table 144: Properties of each product.

Id	Name	SBO
species_8	F6P	
E4P_astrocytes	E4P	

Kinetic Law

Derived unit contains undeclared units

$$v_{54} = \mathrm{vol}\left(\mathrm{compartment\_3}\right) \cdot \mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \frac{\mathrm{species\_10}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{S7P\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{species\_8}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{E4P\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) \tag{223}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{224}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{225}$$

Table 145: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		0.008		☑
K_S1	K_S1		0.168		☑
K_S2	K_S2		0.193		☑
Keq	Keq		0.324		☑
K_P1	K_P1		0.080		☑
K_P2	K_P2		0.110		☑

9.55 Reaction TAL_neurons_R01827

This is a reversible reaction of two reactants forming two products.

Name TAL_neurons (R01827)

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{species\_9} + \mathrm{S7P\_neurons} \rightleftharpoons \mathrm{species\_7} + \mathrm{E4P\_neurons} \tag{226}$$

Reactants

Table 146: Properties of each reactant.

Id	Name	SBO
species_9	GAP	
S7P_neurons	S7P	

Products

Table 147: Properties of each product.

Id	Name	SBO
species_7	F6P	
E4P_neurons	E4P	

Kinetic Law

Derived unit contains undeclared units

$$v_{55} = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \frac{\mathrm{species\_9}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{S7P\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{species\_7}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{E4P\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) \tag{227}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{228}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{229}$$

Table 148: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		0.016		☑
K_S1	K_S1		0.168		☑
K_S2	K_S2		0.193		☑
Keq	Keq		0.324		☑
K_P1	K_P1		0.080		☑
K_P2	K_P2		0.110		☑

9.56 Reaction TKL_2_astrocytes_R01830

This is an irreversible reaction of two reactants forming two products.

Name TKL-2_astrocytes (R01830)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{species\_8} + \text{species\_10} \longrightarrow \text{X5P\_astrocytes} + \text{E4P\_astrocytes} \tag{230}$$

Reactants

Table 149: Properties of each reactant.

Id	Name	SBO
species_8	F6P	
species_10	GAP	

Products

Table 150: Properties of each product.

Id	Name	SBO
X5P_astrocytes	X5P	
E4P_astrocytes	E4P	

Kinetic Law

Derived unit contains undeclared units

$$v_{56} = \mathrm{vol}\left(\mathrm{compartment\_3}\right) \cdot \mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \frac{\mathrm{species\_8}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{species\_10}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{X5P\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \frac{\mathrm{E4P\_astrocytes}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) \tag{231}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{232}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{233}$$

Table 151: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		$1.37124 \cdot 10^{-4}$		☑
K_S1	K_S1		0.080		☑
K_S2	K_S2		0.168		☑
Keq	Keq		0.078		☑
K_P1	K_P1		0.603		☑
K_P2	K_P2		0.110		☑

9.57 Reaction TKL_2_neurons__R01830

This is an irreversible reaction of two reactants forming two products.

Name TKL-2_neurons (R01830)

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{species\_7} + \mathrm{species\_9} \longrightarrow \mathrm{X5P\_neurons} + \mathrm{E4P\_neurons} \tag{234}$$

Reactants

Table 152: Properties of each reactant.

Id	Name	SBO
species_7	F6P	
species_9	GAP	

Products

Table 153: Properties of each product.

Id	Name	SBO
X5P_neurons	X5P	
E4P_neurons	E4P	

Kinetic Law

Derived unit contains undeclared units

$$v_{57} = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \frac{\mathrm{species\_7}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{species\_9}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{X5P\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{E4P\_neurons}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) \tag{235}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{236}$$

$$\mathrm{modular\_rate\_law\_for\_two\_substrates\_\_two\_products}\left(\mathrm{Vmax}, \mathrm{K\_S1}, \mathrm{K\_S2}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{Keq}, \mathrm{K\_P1}, \mathrm{K\_P2}\right) = \mathrm{Vmax} \cdot \frac{1}{\mathrm{K\_S1} \cdot \mathrm{K\_S2}} \cdot \frac{\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}}{\left(1 + \frac{\mathrm{S1}}{\mathrm{K\_S1}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{K\_S2}}\right) + \left(1 + \frac{\mathrm{P1}}{\mathrm{K\_P1}}\right) \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{K\_P2}}\right) - 1} \tag{237}$$

Table 154: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		$2.76758 \cdot 10^{-4}$		☑
K_S1	K_S1		0.080		☑
K_S2	K_S2		0.168		☑
Keq	Keq		0.078		☑
K_P1	K_P1		0.603		☑
K_P2	K_P2		0.110		☑

9.58 Reaction NADPH_oxidase_neurons__R07172

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

Name NADPH oxidase neurons (R07172)

SBO:0000631 pseudoreaction

Reaction equation

$$\text{NADPH\_neurons} \longrightarrow \text{NADP\_neurons} \tag{238}$$

Reactant

Table 155: Properties of each reactant.

Id	Name	SBO
NADPH_neurons	NADPH	

Product

Table 156: Properties of each product.

Id	Name	SBO
NADP_neurons	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{58} = \text{k1} \cdot \text{NADPH\_neurons} \tag{239}$$

Table 157: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$4.23283 \cdot 10^{-4}$		☑

9.59 Reaction NADPH_oxidase_astrocytes__R07172

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

Name NADPH oxidase astrocytes (R07172)

SBO:0000631 pseudoreaction

Reaction equation

$$\text{NADPH\_astrocytes} \longrightarrow \text{NADP\_astrocytes} \tag{240}$$

Reactant

Table 158: Properties of each reactant.

Id	Name	SBO
NADPH_astrocytes	NADPH	

Product

Table 159: Properties of each product.

Id	Name	SBO
NADP_astrocytes	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{59} = \text{k1} \cdot \text{NADPH\_astrocytes} \tag{241}$$

Table 160: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$2.09722 \cdot 10^{-4}$		☑

9.60 Reaction R5P_sink_astrocytes__n_a_

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

Name R5P sink_astrocytes (n.a.)

SBO:0000631 pseudoreaction

Reaction equation

$$\text{R5P\_astrocytes} \longrightarrow \emptyset \tag{242}$$

Reactant

Table 161: Properties of each reactant.

Id	Name	SBO
R5P_astrocytes	R5P	

Kinetic Law

Derived unit contains undeclared units

$$v_{60} = \text{NULL} \cdot \text{R5P\_astrocytes} \tag{243}$$

9.61 Reaction R5P_sink_neurons__n_a_

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

Name R5P sink_neurons (n.a.)

SBO:0000631 pseudoreaction

Reaction equation

$$\text{R5P\_neurons} \longrightarrow \emptyset \tag{244}$$

Reactant

Table 162: Properties of each reactant.

Id	Name	SBO
R5P_neurons	R5P	

Kinetic Law

Derived unit contains undeclared units

$$v_{61} = \mathrm{k1} \cdot \mathrm{R5P\_neurons} \tag{245}$$

Table 163: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.0		☑

9.62 Reaction PGI_astrocytes__R02740___HS

This is a reversible reaction of one reactant forming one product.

Name PGI_astrocytes (R02740) (HS)

Reaction equation

$$\mathrm{species\_6} \rightleftharpoons \mathrm{species\_8} \tag{246}$$

Reactant

Table 164: Properties of each reactant.

Id	Name	SBO
species_6	G6P	

Product

Table 165: Properties of each product.

Id	Name	SBO
species_8	F6P	

Kinetic Law

Derived unit contains undeclared units

$$v_{62} = \mathrm{vol}\left(\mathrm{compartment\_3}\right) \cdot \left(\mathrm{k1} \cdot \frac{\mathrm{species\_6}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)} - \mathrm{k2} \cdot \frac{\mathrm{species\_8}}{\mathrm{vol}\left(\mathrm{compartment\_3}\right)}\right) \tag{247}$$

Table 166: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		931.69		☑
k2	k2		2273.32		☑

9.63 Reaction HK_neurons__R01786___HeinrichSchuster

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

Name HK_neurons (R01786) (HeinrichSchuster)

SBO:0000176 biochemical reaction

Reaction equation

$$\text{species\_3} + \text{species\_1} \xrightarrow{\text{species\_2}} \text{species\_2} + \text{ADP\_neurons} \tag{248}$$

Reactants

Table 167: Properties of each reactant.

Id	Name	SBO
species_3	ATP	
species_1	GLC	

Modifier

Table 168: Properties of each modifier.

Id	Name	SBO
species_2	G6P	

Products

Table 169: Properties of each product.

Id	Name	SBO
species_2	G6P	
ADP_neurons	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{63} = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{vHK\_\_HS}\left(\mathrm{k\_HK}, \frac{\mathrm{species\_3}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \frac{\mathrm{species\_2}}{\mathrm{vol}\left(\mathrm{compartment\_2}\right)}, \mathrm{K\_I\_G6P}\right) \tag{249}$$

$$\mathrm{vHK\_\_HS}\left(\mathrm{k\_HK}, \mathrm{ATP}, \mathrm{G6P}, \mathrm{K\_I\_G6P}\right) = \mathrm{k\_HK} \cdot \mathrm{ATP} \cdot \left(1 + \frac{\mathrm{G6P}}{\mathrm{K\_I\_G6P}}\right)^{1} \tag{250}$$

$$\mathrm{vHK\_\_HS}\left(\mathrm{k\_HK}, \mathrm{ATP}, \mathrm{G6P}, \mathrm{K\_I\_G6P}\right) = \mathrm{k\_HK} \cdot \mathrm{ATP} \cdot \left(1 + \frac{\mathrm{G6P}}{\mathrm{K\_I\_G6P}}\right)^{1} \tag{251}$$

Table 170: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_HK	k_HK		0.022		☑
K_I_G6P	K_I_G6P		0.020		☑

9.64 Reaction PGI_neurons__R02740___HS

This is a reversible reaction of one reactant forming one product.

Name PGI_neurons (R02740) (HS)

Reaction equation

$$\mathrm{species\_2} \rightleftharpoons \mathrm{species\_7} \tag{252}$$

Reactant

Table 171: Properties of each reactant.

Id	Name	SBO
species_2	G6P	

Product

Table 172: Properties of each product.

Id	Name	SBO
species_7	F6P	

Kinetic Law

Derived unit contains undeclared units

$$v_{64} = \mathrm{vol}\,(\mathrm{compartment\_2}) \cdot \left(\mathrm{k1} \cdot \frac{\mathrm{species\_2}}{\mathrm{vol}\,(\mathrm{compartment\_2})} - \mathrm{k2} \cdot \frac{\mathrm{species\_7}}{\mathrm{vol}\,(\mathrm{compartment\_2})} \right) \quad (253)$$

Table 173: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		931.69		☑
k2	k2		2273.32		☑

10 Derived Rate Equations

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

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.

10.1 Species species_23

Name O2

Initial amount 0.040323291746644 mmol

This species takes part in four reactions (as a reactant in O2_exchange_capillary_neurons, O2_exchange_capillary_astrocytes and as a product in Blood_flow_contribution_to_capillary_O2 and as a modifier in inflow_of_dHb).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_23} = v_{20} - v_{18} - v_{19} \quad (254)$$

10.2 Species species_24

Name CO2

Initial amount 0.0121467082533562 mmol

This species takes part in three reactions (as a reactant in Flow_of_CO2_between_capillary-_and_vessel__artery_ and as a product in reaction_13, reaction_14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_24} = 3\,v_8 + 3\,v_9 - v_{23} \tag{255}$$

10.3 Species species_25

Name GLC

Initial amount 0.0253903826849856 mmol

This species takes part in three reactions (as a reactant in reaction_19, reaction_20 and as a product in Blood_flow_contribution_to_capillary_GLC).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_25} = v_{21} - v_{12} - v_{13} \tag{256}$$

10.4 Species species_26

Name LAC

Initial amount 0.00188912996259375 mmol

This species takes part in three reactions (as a reactant in Blood_flow_contribution_to-_capillary_LAC and as a product in reaction_21, reaction_24).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_26} = v_{14} + v_{17} - v_{22} \tag{257}$$

10.5 Species dHb

Name dHb

Initial amount $2.62913971209081 \cdot 10^{-4}$ mmol

This species takes part in two reactions (as a reactant in outflow_of_dHb and as a product in inflow_of_dHb).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{dHb} = v_{32} - v_{33} \tag{258}$$

10.6 Species species_1

Name GLC

Initial amount 0.513125204430911 mmol

This species takes part in two reactions (as a reactant in HK_neurons__R01786___HeinrichSchuster and as a product in reaction_17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_1} = v_{10} - v_{63} \tag{259}$$

10.7 Species species_2

Name G6P

Initial amount 0.0506867341754652 mmol

This species takes part in four reactions (as a reactant in ZWF_neurons__R02736, PGI_neurons__R02740___HS and as a product in HK_neurons__R01786___HeinrichSchuster and as a modifier in HK_neurons__R01786___HeinrichSchuster).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_2} = v_{63} - v_{43} - v_{64} \tag{260}$$

10.8 Species species_3

Name ATP

Initial amount 1.01756735100076 mmol

This species takes part in nine reactions (as a reactant in reaction_5, vPUMP_neurons, ATPase_neurons, HK_neurons__R01786___HeinrichSchuster and as a product in reaction_7, reaction_9, reaction_13, AK_neurons, CK_neurons_forward__R01881).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_3} = v_4 + v_6 + 15\,v_8 + v_{36} + v_{39} - v_2 - v_{24} - v_{34} - v_{63} \tag{261}$$

10.9 Species species_7

Name F6P

Initial amount 0.0207718119329183 mmol

This species takes part in four reactions (as a reactant in reaction_5, TKL_2_neurons__R01830 and as a product in TAL_neurons__R01827, PGI_neurons__R02740___HS).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_7} = v_{55} + v_{64} - v_2 - v_{57} \tag{262}$$

10.10 Species species_9

Name GAP

Initial amount $4.84856903277021 \cdot 10^{-4}$ mmol

This species takes part in five reactions (as a reactant in reaction_7, TAL_neurons__R01827, TKL_2_neurons__R01830 and as a product in reaction_5, TKL_1_neurons__R01641).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_9} = 2\,v_2 + v_{53} - v_4 - v_{55} - v_{57} \tag{263}$$

10.11 Species species_11

Name NADH

Initial amount 0.00736369051750214 mmol

This species takes part in three reactions (as a reactant in reaction_13, LDH_neurons_forward__R00703 and as a product in reaction_7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_11} = v_4 - v_8 - v_{41} \tag{264}$$

10.12 Species species_12

Name PEP

Initial amount 0.00137130155845014 mmol

This species takes part in two reactions (as a reactant in reaction_9 and as a product in reaction_7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_12} = v_4 - v_6 \tag{265}$$

10.13 Species species_15

Name PYR

Initial amount 0.05894677979576 mmol

This species takes part in three reactions (as a reactant in reaction_13, LDH_neurons_forward__R00703 and as a product in reaction_9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_15} = v_6 - v_8 - v_{41} \tag{266}$$

10.14 Species species_18

Name LAC

Initial amount 0.631465311475557 mmol

This species takes part in two reactions (as a product in reaction_22, LDH_neurons_forward__R00703).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_18} = v_{15} + v_{41} \tag{267}$$

10.15 Species species_16

Name O2

Initial amount 0.0134379352275963 mmol

This species takes part in two reactions (as a reactant in reaction_13 and as a product in O2_exchange_capillary_neurons).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_16} = v_{18} - 3\,v_{8} \tag{268}$$

10.16 Species species_21

Name PCr

Notes Phosphocreatine

Initial amount 0.648285185366582 mmol

This species takes part in one reaction (as a reactant in CK_neurons_forward__R01881).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_21} = -v_{39} \tag{269}$$

10.17 Species Na__neurons

Name Na+

Initial amount 6.98905574867159 mmol

This species takes part in three reactions (as a reactant in vPUMP_neurons and as a product in vLEAK_Na_neurons, vSTIM).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Na\_\_neurons} = v_{26} + v_{28} - 3\,v_{24} \tag{270}$$

10.18 Species GLU_neurons

Name GLU

Initial amount 1.35000000000001 mmol

This species takes part in two reactions (as a reactant in vGLU_ne and as a product in vGLU_gn).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLU\_neurons} = v_{31} - v_{29} \tag{271}$$

10.19 Species ADP_neurons

Name ADP

Initial amount 0.0502819665719672 mmol

This species takes part in nine reactions (as a reactant in reaction_7, reaction_9, reaction_13, AK_neurons, CK_neurons_forward__R01881 and as a product in reaction_5, vPUMP_neurons, ATPase_neurons, HK_neurons__R01786___HeinrichSchuster).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP\_neurons} = v_2 + v_{24} + v_{34} + v_{63} - v_4 - v_6 - 15\,v_8 - 2\,v_{36} - v_{39} \tag{272}$$

10.20 Species AMP_neurons

Name AMP

Initial amount 0.00270068242727579 mmol

Initial assignment AMP_neurons

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP\_neurons} = v_{36} \tag{273}$$

10.21 Species Cr_neurons

Name Cr

Initial amount 1.60171481463342 mmol

Initial assignment Cr_neurons

This species takes part in one reaction (as a product in CK_neurons_forward__R01881).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cr\_neurons} = v_{39} \tag{274}$$

10.22 Species NAD_neurons

Name NAD

Initial amount 0.0916363094824979 mmol

Initial assignment NAD_neurons

This species takes part in three reactions (as a reactant in reaction_7 and as a product in reaction_13, LDH_neurons_forward__R00703).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD\_neurons} = v_8 + v_{41} - v_4 \tag{275}$$

10.23 Species G6L_neurons

Name G6L

Initial amount $1.35054620762897 \cdot 10^{-6}$ mmol

This species takes part in two reactions (as a reactant in SOL_neurons__R02035 and as a product in ZWF_neurons__R02736).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G6L\_neurons} = v_{43} - v_{44} \tag{276}$$

10.24 Species P6G_neurons

Name P6G

Initial amount 0.00129746785673949 mmol

This species takes part in two reactions (as a reactant in GND_neurons___R01528 and as a product in SOL_neurons__R02035).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P6G\_neurons} = v_{44} - v_{46} \tag{277}$$

10.25 Species Ru5P_neurons

Name Ru5P

Initial amount $3.03470299804797 \cdot 10^{-4}$ mmol

This species takes part in three reactions (as a reactant in RPE_neurons__R01529, RKI_neurons__R01056 and as a product in GND_neurons___R01528).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ru5P\_neurons} = v_{46} - v_{48} - v_{51} \tag{278}$$

10.26 Species X5P_neurons

Name X5P

Initial amount 0.00930686571830458 mmol

This species takes part in three reactions (as a reactant in TKL_1_neurons__R01641 and as a product in RPE_neurons__R01529, TKL_2_neurons__R01830).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X5P\_neurons} = v_{48} + v_{57} - v_{53} \tag{279}$$

10.27 Species R5P_neurons

Name R5P

Initial amount $1.21527766162824 \cdot 10^{-5}$ mmol

This species takes part in three reactions (as a reactant in TKL_1_neurons__R01641, R5P_sink_neurons__n_a_ and as a product in RKI_neurons__R01056).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R5P\_neurons} = v_{51} - v_{53} - v_{61} \tag{280}$$

10.28 Species S7P_neurons

Name S7P

Initial amount 0.519857938505835 mmol

This species takes part in two reactions (as a reactant in TAL_neurons__R01827 and as a product in TKL_1_neurons__R01641).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S7P\_neurons} = v_{53} - v_{55} \tag{281}$$

10.29 Species E4P_neurons

Name E4P

Initial amount 0.00293045545188872 mmol

This species takes part in two reactions (as a product in TAL_neurons__R01827, TKL_2_neurons__R01830).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E4P\_neurons} = v_{55} + v_{57} \tag{282}$$

10.30 Species NADPH_neurons

Name NADPH

Initial amount 0.13105170046902 mmol

This species takes part in three reactions (as a reactant in NADPH_oxidase_neurons__R07172 and as a product in ZWF_neurons__R02736, GND_neurons___R01528).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH\_neurons} = v_{43} + v_{46} - v_{58} \tag{283}$$

10.31 Species NADP_neurons

Name NADP

Initial amount $9.96586007623714 \cdot 10^{-10}$ mmol

This species takes part in three reactions (as a reactant in ZWF_neurons__R02736, GND_neurons-___R01528 and as a product in NADPH_oxidase_neurons__R07172).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADP\_neurons} = v_{58} - v_{43} - v_{46} \tag{284}$$

10.32 Species species_4

Name GLC

Initial amount 0.28506553827656 mmol

This species takes part in three reactions (as a reactant in reaction_2 and as a product in reaction_18, reaction_20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_4} = v_{11} + v_{13} - v_{1} \tag{285}$$

10.33 Species species_5

Name ATP

Initial amount 0.453875749582273 mmol

This species takes part in ten reactions (as a reactant in reaction_2, reaction_6, vPUMP-_astrocytes, vGLU_gn, ATPase_astrocytes and as a product in reaction_8, reaction_10, reaction_14, AK_astrocytes, CK_astrocytes_forward__R01881).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_5} = v_{5} + v_{7} + 15\,v_{9} + v_{37} + v_{38} - v_{1} - v_{3} - v_{25} - v_{31} - v_{35} \tag{286}$$

10.34 Species species_6

Name G6P

Initial amount 0.0170326696107673 mmol

This species takes part in four reactions (as a reactant in ZWF_astrocytes__R02736, PGI_astrocytes__R02740___HS and as a product in reaction_2 and as a modifier in reaction_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_6} = v_1 - v_{42} - v_{62} \tag{287}$$

10.35 Species species_8

Name F6P

Initial amount 0.00698016362763041 mmol

This species takes part in four reactions (as a reactant in reaction_6, TKL_2_astrocytes__R01830 and as a product in TAL_astrocytes__R01827, PGI_astrocytes__R02740___HS).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_8} = v_{54} + v_{62} - v_3 - v_{56} \tag{288}$$

10.36 Species species_10

Name GAP

Initial amount $5.51039449892962 \cdot 10^{-4}$ mmol

This species takes part in five reactions (as a reactant in reaction_8, TAL_astrocytes__R01827, TKL_2_astrocytes__R01830 and as a product in reaction_6, TKL_1_astrocytes__R01641).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_10} = 2\,v_3 + v_{52} - v_5 - v_{54} - v_{56} \tag{289}$$

10.37 Species species_13

Name NADH

Initial amount 0.014484722086168 mmol

This species takes part in three reactions (as a reactant in reaction_14, LDH_astrocytes_forward__R00703 and as a product in reaction_8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_13} = v_5 - v_9 - v_{40} \tag{290}$$

10.38 Species species_14

Name PEP

Initial amount $2.31197219260613 \cdot 10^{-4}$ mmol

This species takes part in two reactions (as a reactant in reaction_10 and as a product in reaction_8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_14} = v_5 - v_7 \tag{291}$$

10.39 Species species_17

Name PYR

Initial amount 0.0391626309395164 mmol

This species takes part in three reactions (as a reactant in reaction_14, LDH_astrocytes_forward__R00703 and as a product in reaction_10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_17} = v_7 - v_9 - v_{40} \tag{292}$$

10.40 Species species_19

Name LAC

Initial amount 0.341202758724066 mmol

This species takes part in three reactions (as a reactant in reaction_23, reaction_24 and as a product in LDH_astrocytes_forward__R00703).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_19} = v_{40} - v_{16} - v_{17} \tag{293}$$

10.41 Species species_20

Name O2

Initial amount 0.0114703177351059 mmol

This species takes part in two reactions (as a reactant in reaction_14 and as a product in O2_exchange_capillary_astrocytes).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_20} = v_{19} - 3\,v_9 \tag{294}$$

10.42 Species species_22

Name PCr

Notes Phosphocreatine

Initial amount 0.0943080249454476 mmol

This species takes part in one reaction (as a reactant in CK_astrocytes_forward__R01881).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_22} = -\,v_{38} \tag{295}$$

10.43 Species Na__astrocytes

Name Na+

Initial amount 4.00737645868716 mmol

This species takes part in three reactions (as a reactant in vPUMP_astrocytes and as a product in vLEAK_Na_astrocytes, vGLU_eg).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Na\_\_astrocytes} = v_{27} + v_{30} - 3\,v_{25} \tag{296}$$

10.44 Species GLU_astrocytes

Name GLU

Initial amount 0 mmol

This species takes part in two reactions (as a reactant in vGLU_gn and as a product in vGLU_eg).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{GLU\_astrocytes} = v_{30} - v_{31} \tag{297}$$

10.45 Species ADP_astrocytes

Name ADP

Initial amount 0.111239857216292 mmol

This species takes part in ten reactions (as a reactant in reaction_8, reaction_10, reaction_14, AK_astrocytes, CK_astrocytes_forward__R01881 and as a product in reaction_2, reaction_6, vPUMP_astrocytes, vGLU_gn, ATPase_astrocytes).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{ADP\_astrocytes} = v_1 + v_3 + v_{25} + v_{31} + v_{35} - v_5 - v_7 - 15\,v_9 - 2\,v_{37} - v_{38} \tag{298}$$

10.46 Species AMP_astrocytes

Name AMP

Initial amount 0.0296343932014343 mmol

Initial assignment AMP_astrocytes

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP\_astrocytes} = v_{37} \tag{299}$$

10.47 Species Cr_astrocytes

Name Cr

Initial amount 1.15569197505455 mmol

Initial assignment Cr_astrocytes

This species takes part in one reaction (as a product in CK_astrocytes_forward__R01881).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cr\_astrocytes} = v_{38} \tag{300}$$

10.48 Species NAD_astrocytes

Name NAD

Initial amount 0.040515277913832 mmol

Initial assignment NAD_astrocytes

This species takes part in three reactions (as a reactant in reaction_8 and as a product in reaction_14, LDH_astrocytes_forward__R00703).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD\_astrocytes} = v_9 + v_{40} - v_5 \tag{301}$$

10.49 Species G6L_astrocytes

Name G6L

Initial amount $7.49440003798258 \cdot 10^{-7}$ mmol

This species takes part in two reactions (as a reactant in SOL_astrocytes__R02035 and as a product in ZWF_astrocytes__R02736).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G6L\_astrocytes} = v_{42} - v_{45} \tag{302}$$

10.50 Species P6G_astrocytes

Name P6G

Initial amount $4.50905835212361 \cdot 10^{-4}$ mmol

This species takes part in two reactions (as a reactant in GND_astrocytes__R01528 and as a product in SOL_astrocytes__R02035).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P6G\_astrocytes} = v_{45} - v_{47} \tag{303}$$

10.51 Species Ru5P_astrocytes

Name Ru5P

Initial amount $1.68586812670336 \cdot 10^{-4}$ mmol

This species takes part in three reactions (as a reactant in RPE_astrocytes__R01529, RKI_astrocytes__R01056 and as a product in GND_astrocytes__R01528).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ru5P\_astrocytes} = v_{47} - v_{49} - v_{50} \tag{304}$$

10.52 Species X5P_astrocytes

Name X5P

Initial amount 0.00517018155675064 mmol

This species takes part in three reactions (as a reactant in TKL_1_astrocytes__R01641 and as a product in RPE_astrocytes__R01529, TKL_2_astrocytes__R01830).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X5P\_astrocytes} = v_{49} + v_{56} - v_{52} \tag{305}$$

10.53 Species R5P_astrocytes

Name R5P

Initial amount $6.5024908937442 \cdot 10^{-6}$ mmol

This species takes part in three reactions (as a reactant in TKL_1_astrocytes__R01641, R5P_sink_astrocytes__n_a_ and as a product in RKI_astrocytes__R01056).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R5P\_astrocytes} = v_{50} - v_{52} - v_{60} \tag{306}$$

10.54 Species S7P_astrocytes

Name S7P

Initial amount 0.0691726529321511 mmol

This species takes part in two reactions (as a reactant in TAL_astrocytes__R01827 and as a product in TKL_1_astrocytes__R01641).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S7P\_astrocytes} = v_{52} - v_{54} \tag{307}$$

10.55 Species E4P_astrocytes

Name E4P

Initial amount 0.00142484578792443 mmol

This species takes part in two reactions (as a product in TAL_astrocytes__R01827, TKL_2-_astrocytes__R01830).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E4P\_astrocytes} = v_{54} + v_{56} \tag{308}$$

10.56 Species NADP_astrocytes

Name NADP

Initial amount $6.89248119909569 \cdot 10^{-10}$ mmol

This species takes part in three reactions (as a reactant in ZWF_astrocytes__R02736, GND-_astrocytes__R01528 and as a product in NADPH_oxidase_astrocytes__R07172).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADP\_astrocytes} = v_{59} - v_{42} - v_{47} \tag{309}$$

10.57 Species NADPH_astrocytes

Name NADPH

Initial amount 0.0728065001051474 mmol

This species takes part in three reactions (as a reactant in NADPH_oxidase_astrocytes_-_R07172 and as a product in ZWF_astrocytes__R02736, GND_astrocytes__R01528).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH\_astrocytes} = v_{42} + v_{47} - v_{59} \tag{310}$$

10.58 Species species_27

Name GLC

Initial amount 0.228060016230605 mmol

This species takes part in three reactions (as a reactant in reaction_17, reaction_18 and as a product in reaction_19).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_27} = v_{12} - v_{10} - v_{11} \tag{311}$$

10.59 Species species_28

Name LAC

Initial amount 0.269553776630414 mmol

This species takes part in three reactions (as a reactant in reaction_21, reaction_22 and as a product in reaction_23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_28} = v_{16} - v_{14} - v_{15} \tag{312}$$

10.60 Species GLU_extracellular_space

Name GLU

Initial amount 0 mmol

This species takes part in two reactions (as a reactant in vGLU_eg and as a product in vGLU_ne).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{GLU\_extracellular\_space} = v_{29} - v_{30} \tag{313}$$

10.61 Species Na__extracellular_space

Name Na+

Initial amount 30 mmol

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Na\_\_extracellular\_space} = 0 \tag{314}$$

10.62 Species O2_artery

Name O2

Initial amount 0.0458700000000001 mmol

This species takes part in two reactions (as a reactant in Blood_flow_contribution_to_capillary_O2 and as a modifier in inflow_of_dHb), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{O2\_artery} = 0 \tag{315}$$

10.63 Species CO2_artery

Name CO2

Initial amount 0.00660000000000004 mmol

This species takes part in one reaction (as a product in Flow_of_CO2_between_capillary_and_vessel__artery_), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2\_artery} = 0 \tag{316}$$

10.64 Species GLC_artery

Name GLC

Initial amount 0.0264000000000002 mmol

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLC\_artery} = 0 \tag{317}$$

10.65 Species LAC_artery

Name LAC

Initial amount 0.0017215 mmol

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{LAC\_artery} = 0 \tag{318}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000176 biochemical reaction: An event involving one or more chemical entities that modifies the electrochemical structure of at least one of the participants.

SBO:0000185 transport reaction: Movement of a physical entity without modification of the structure of the entity

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

SBO:0000395 encapsulating process: An aggregation of interactions and entities into a single process

SBO:0000631 pseudoreaction: A conceptual process used for modeling purposes, often created solely to complete model structure, with respect to providing inflow or outflow of matter or material. Unlike other reactions, pseudoreactions are not usually subjected to mass balance considerations

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