SBML Model Report

Model name: “Sass2009 - Approach to an -synuclein-based BST model of Parkinson’s disease”

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Audald Lloret i Villas[1] at April thirteenth 2015 at 5:26 p. m. and last time modified at April 14th 2015 at 2:38 p. m. Table 1 gives an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	5
species types	0	species	76
events	0	constraints	0
reactions	58	function definitions	7
global parameters	245	unit definitions	3
rules	13	initial assignments	0

Model Notes

Sass2009 - Approach to an-synuclein-based BST model of Parkinson’s disease

This model is described in the article:A pragmatic approach to biochemical systems theory applied to an alpha-synuclein-based model of Parkinson’s disease.Sass MB, Lorenz AN, Green RL, Coleman RA.J. Neurosci. Methods 2009 Apr; 178(2): 366-377

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Abstract:

This paper presents a detailed systems model of Parkinson's disease (PD), developed utilizing a pragmatic application of biochemical systems theory (BST) intended to assist experimentalists in the study of system behavior. This approach utilizes relative values as a reasonable initial estimate for BST and provides a theoretical means of applying numerical solutions to qualitative and semi-quantitative understandings of cellular pathways and mechanisms. The approach allows for the simulation of human disease through its ability to organize and integrate existing information about metabolic pathways without having a full quantitative description of those pathways, so that hypotheses about individual processes may be tested in a systems environment. Incorporating this method, the PD model describes alpha-synuclein aggregation as mediated by dopamine metabolism, the ubiquitin-proteasome system, and lysosomal degradation, allowing for the examination of dynamic pathway interactions and the evaluation of possible toxic mechanisms in the aggregation process. Four system perturbations: elevated alpha-synuclein aggregation, impaired dopamine packaging, increased neurotoxins, and alpha-synuclein overexpression, were analyzed for correlation to qualitative PD system hypotheses present in the literature, with the model demonstrating a high level of agreement with these hypotheses. Additionally, various PD treatment methods, including levadopa and monoamine oxidase inhibition (MAOI) therapy, were applied to the disease models to examine their effects on the system. Future additions and refinements to the model may further the understanding of the emergent behaviors of the disease, helping in the identification of system sensitivities and possible therapeutic targets.

This model is hosted on BioModels Database and identified by: BIOMD0000000575.

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 two are predefined by SBML and not mentioned in the model.

2.1 Unit `volume`

Name volume

Definition dimensionless

2.2 Unit `time`

Name time

Definition dimensionless

2.3 Unit substance

Name substance

Definition dimensionless

2.4 Unit area

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

Definition m^2

2.5 Unit length

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

Definition m

3 Compartments

This model contains five compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
Neuronal_cytosol	Neuronal cytosol		3	1	dimensionless	☑	
Vesicle	Vesicle		3	1	dimensionless	☑	
Autophagosome	Autophagosome		3	1	dimensionless	☑	
Proteasome	Proteasome		3	1	dimensionless	☑	
Lysosome	Lysosome		3	1	dimensionless	☑	

3.1 Compartment Neuronal_cytosol

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

Name Neuronal cytosol

3.2 Compartment Vesicle

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

Name Vesicle

3.3 Compartment Autophagosome

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

Name Autophagosome

3.4 Compartment `Proteasome`

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

Name Proteasome

3.5 Compartment `Lysosome`

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

Name Lysosome

4 Species

This model contains 76 species. The boundary condition of 28 of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 9 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
`Protofibril`	Protofibril	`Neuronal_cytosol`	dimensionless · dimensionless^{-1}	⊟	⊟
`Fibril`	Fibril	`Neuronal_cytosol`	dimensionless · dimensionless^{-1}	⊟	⊟
`Lewy_body`	Lewy_body	`Neuronal_cytosol`	dimensionless · dimensionless^{-1}	⊟	⊟
`Dopamine`	Dopamine	`Neuronal_cytosol`	dimensionless · dimensionless^{-1}	⊟	⊟
`OH`	OH-	`Neuronal_cytosol`	dimensionless · dimensionless^{-1}	⊟	⊟
`OH_radical`	OH_radical	`Neuronal_cytosol`	dimensionless · dimensionless^{-1}	⊟	⊟
`H2O2`	H2O2	`Neuronal_cytosol`	dimensionless · dimensionless^{-1}	⊟	⊟
`DA_quinone`	DA_quinone	`Neuronal_cytosol`	dimensionless · dimensionless^{-1}	⊟	⊟
`Ubiquitin`	Ubiquitin	`Neuronal_cytosol`	dimensionless · dimensionless^{-1}	⊟	⊟
`E1`	E1	`Neuronal_cytosol`	dimensionless · dimensionless^{-1}	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
Ub_E1	Ub-E1	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
UbcH8	UbcH8	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
UbcH8_Ub	UbcH8-Ub	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Parkin	Parkin	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Parkin_sub	Parkin-sub	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Parkin_synphilin-_1	Parkin-synphilin-1	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Parkin_synphilin-_1_ub	Parkin-synphilin-1-ub	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Parkin_sub_ub4	Parkin-sub-ub4	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Fragments	Fragments	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
UCH_L1	UCH-L1	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
L_Dopa	L-Dopa	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
DOPAL	DOPAL	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
DOPAC	DOPAC	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
GSH	GSH	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
GSSG	GSSG	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Fe2	Fe2+	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	☑
Fe3	Fe3+	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
UbcH8ub2	UbcH8ub2	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
UbcH8ub3	UbcH8ub3	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
UbcH8ub4	UbcH8ub4	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
UbcH13_Uev1a	UbcH13/Uev1a	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
asyn_UCH_L1	asyn-UCH-L1	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
asyn_ub	asyn-ub	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Protofibril_UCH-_L1	Protofibril-UCH-L1	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Protofibril_Ub	Protofibril-Ub	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Hsc70_asyn	Hsc70-asyn	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Hsc70_Protofibril	Hsc70-Protofibril	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Hsc70_fibril	Hsc70-fibril	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Hsc70	Hsc70	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
DA_S_parkin	DA-S-parkin	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
O2	O2-	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
DA_GSH	DA-GSH	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Neuromelanin	Neuromelanin	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Neuromelanin-_ntox_Fe3	Neuromelanin-ntox-Fe3+	Neuronal_cytosol	dimensionless · dimensionless^{-1}	⊟	⊟
Alpha_synuclein	Alpha_synuclein	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
ATP	ATP	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
Synphilin_1	Synphilin-1	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
Substrate	Substrate	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
TH	TH	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
L_Tyr	L-Tyr	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
CO2	CO2	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
Neurotoxins	Neurotoxins	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
Bioamines	Bioamines	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
VMAT2	VMAT2	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
O2_0	O2	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
MAO	MAO	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
NH3	NH3	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
ALDH	ALDH	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
NAD	NAD+	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
NADH	NADH	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
Catalase	Catalase	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
H2O	H2O	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
Gluta_per	Gluta_per	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
Gluta_red	Gluta_red	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
DDC	DDC	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
Preautophagosome-_membrane	Preautophagosome_membrane	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
SOD	SOD	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
Cysteine	Cysteine	Neuronal_cytosol	dimensionless · dimensionless^{-1}	☑	☑
V_DA	V-DA	Vesicle	dimensionless · dimensionless^{-1}	⊟	⊟
V_ntox_ba	V-ntox-ba	Vesicle	dimensionless · dimensionless^{-1}	⊟	⊟
Vesicle_0	Vesicle	Vesicle	dimensionless · dimensionless^{-1}	☑	☑
Autophagosome_0	Autophagosome	Autophagosome	dimensionless · dimensionless^{-1}	⊟	⊟
Proteasome_0	Proteasome	Proteasome	dimensionless · dimensionless^{-1}	☑	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
Lysosome_0	Lysosome	Lysosome	dimensionless · dimensionless^{-1}	☑	☑

5 Parameters

This model contains 245 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
g11	g11		1.000		☑
p186	p186		0.500		☑
p110	p110		1.000		☑
p19	p19		1.000		☑
p18	p18		1.000		☑
k1	k1		0.030		☑
g22	g22		1.000		☑
p286	p286		0.250		☑
p210	p210		0.500		☑
p29	p29		0.500		☑
p28	p28		0.500		☑
i26	i26		−1.000		☑
k2	k2		0.010		☑
g326	g326		1.000		☑
g23	g23		1.000		☑
k3	k3		0.007		☑
k4	k4		0.900		☑
i41	i41		−0.010		☑
i42	i42		−0.010		☑
i43	i43		−0.010		☑
g412	g412		1.000		☑
g415	g415		1.000		☑
g427	g427		1.000		☑
g430	g430		1.000		☑
k6	k6		0.500		☑
g613	g613		1.000		☑
g614	g614		1.000		☑
g615	g615		1.000		☑
k7	k7		0.030		☑
g715	g715		1.000		☑
g716	g716		1.000		☑
g717	g717		1.000		☑
k8	k8		0.001		☑
g819	g819		1.000		☑
g821	g821		1.000		☑
k9	k9		0.001		☑
g919	g919		1.000		☑

Id	Name	SBO	Value	Unit	Constant
g920	g920		1.000		☑
k10	k10		0.050		☑
g1025	g1025		1.000		☑
g1072	g1072		1.000		☑
k11	k11		0.050		☑
g1124	g1124		1.000		☑
g1170	g1170		1.000		☑
k13	k13		0.100		☑
i131	i131		−0.010		☑
i1310	i1310		−0.010		☑
g1335	g1335		1.000		☑
g1336	g1336		1.000		☑
g1351	g1351		1.000		☑
k14	k14		3.000		☑
g1437	g1437		1.000		☑
g1467	g1467		1.000		☑
k15	k15		0.200		☑
i152	i152		−0.100		☑
g156	g156		1.000		☑
g1544	g1544		1.000		☑
g1545	g1545		1.000		☑
k16	k16		10^{-4}		☑
g1643	g1643		1.000		☑
g1644	g1644		1.000		☑
k17	k17		10^{-4}		☑
g1742	g1742		1.000		☑
g1744	g1744		1.000		☑
k18	k18		0.020		☑
g186	g186		1.000		☑
g1851	g1851		1.000		☑
k19	k19		0.010		☑
g196	g196		1.000		☑
g1951	g1951		1.000		☑
g1953	g1953		1.000		☑
g1960	g1960		1.000		☑
k20	k20		0.100		☑
g209	g209		1.000		☑
g2065	g2065		1.000		☑
k21	k21		0.100		☑
g2166	g2166		1.000		☑
k22	k22		0.500		☑
g229	g229		1.000		☑

Id	Name	SBO	Value	Unit	Constant
g2259	g2259		1.000		☑
k23	k23		0.500		☑
g239	g239		1.000		☑
g2361	g2361		1.000		☑
g2362	g2362		1.000		☑
k24	k24		1.000		☑
g2463	g2463		1.000		☑
g2464	g2464		1.000		☑
k25	k25		0.050		☑
g2552	g2552		1.000		☑
g2555	g2555		0.300		☑
g2556	g2556		0.250		☑
k26f	k26f		0.050		☑
g26f15	g26f15		1.000		☑
g26f16	g26f16		1.000		☑
g26f18	g26f18		1.000		☑
k26r	k26r		0.005		☑
g26r30	g26r30		1.000		☑
g26r68	g26r68		1.000		☑
k27f	k27f		0.050		☑
g27f15	g27f15		1.000		☑
g27f16	g27f16		1.000		☑
g27f68	g27f68		1.000		☑
k27r	k27r		0.005		☑
g27r30	g27r30		1.000		☑
g27r69	g27r69		1.000		☑
k28f	k28f		0.050		☑
g28f15	g28f15		1.000		☑
g28f16	g28f16		1.000		☑
g28f69	g28f69		1.000		☑
k28r	k28r		0.005		☑
g28r30	g28r30		1.000		☑
g28r70	g28r70		1.000		☑
k29	k29		0.050		☑
g2915	g2915		1.000		☑
g2916	g2916		1.000		☑
g2971	g2971		1.000		☑
k30	k30		0.001		☑
g301	g301		1.000		☑
g3030	g3030		1.000		☑
k31	k31		0.050		☑
g3172	g3172		1.000		☑

Id	Name	SBO	Value	Unit	Constant
g3173	g3173		1.000		☑
k32	k32		0.001		☑
g321	g321		1.000		☑
p328	p328		0.100		☑
p329	p329		0.100		☑
p3210	p3210		0.100		☑
p3286	p3286		0.050		☑
g3274	g3274		1.000		☑
k33	k33		0.001		☑
g332	g332		1.000		☑
g3330	g3330		1.000		☑
k34	k34		0.050		☑
g3472	g3472		1.000		☑
g3475	g3475		1.000		☑
k35	k35		0.001		☑
g352	g352		1.000		☑
p358	p358		0.100		☑
p359	p359		0.100		☑
p3510	p3510		0.100		☑
p3586	p3586		0.050		☑
g3576	g3576		1.000		☑
k36	k36		0.050		☑
i368	i368		−0.100		☑
i369	i369		−0.100		☑
i3610	i3610		−0.100		☑
i3686	i3686		−0.050		☑
g3677	g3677		1.000		☑
g3679	g3679		1.000		☑
k37	k37		0.050		☑
g3770	g3770		1.000		☑
g3773	g3773		1.000		☑
k38	k38		0.700		☑
i381	i381		−0.010		☑
i382	i382		−0.010		☑
i383	i383		−0.010		☑
g3812	g3812		1.000		☑
g3815	g3815		1.000		☑
g3830	g3830		1.000		☑
g3878	g3878		1.000		☑
k43	k43		0.050		☑
g431	g431		1.000		☑
g4384	g4384		1.000		☑

Id	Name	SBO	Value	Unit	Constant
k44	k44		0.045		☑
g442	g442		1.000		☑
g4484	g4484		1.000		☑
k45	k45		0.040		☑
g453	g453		1.000		☑
g4584	g4584		1.000		☑
k46	k46		0.030		☑
i468	i468		−0.100		☑
i469	i469		−0.100		☑
i4610	i4610		−0.100		☑
i4686	i4686		−0.050		☑
g4677	g4677		1.000		☑
g4681	g4681		1.000		☑
k47	k47		0.030		☑
i478	i478		−0.100		☑
i479	i479		−0.100		☑
i4710	i4710		−0.100		☑
i4786	i4786		−0.050		☑
g4777	g4777		1.000		☑
g4782	g4782		1.000		☑
k48	k48		0.030		☑
i488	i488		−0.100		☑
i489	i489		−0.100		☑
i4810	i4810		−0.100		☑
i4886	i4886		−0.050		☑
g4877	g4877		1.000		☑
g4883	g4883		1.000		☑
k50	k50		0.050		☑
g501	g501		1.000		☑
g5080	g5080		1.000		☑
k51	k51		0.050		☑
g512	g512		1.000		☑
g5180	g5180		1.000		☑
k52	k52		0.050		☑
g523	g523		1.000		☑
g5280	g5280		1.000		☑
k53	k53		0.050		☑
g534	g534		1.000		☑
g5380	g5380		1.000		☑
k54	k54		0.005		☑
g5410	g5410		1.000		☑
g5419	g5419		1.000		☑

Id	Name	SBO	Value	Unit	Constant
k55	k55		0.050		☑
g556	g556		1.000		☑
g5586	g5586		1.000		☑
k56	k56		0.050		☑
g5686	g5686		1.000		☑
g5687	g5687		1.000		☑
k57	k57		0.005		☑
g5710	g5710		1.000		☑
g5762	g5762		1.000		☑
k100	k100		0.005		☑
g10037	g10037		1.000		☑
g10051	g10051		1.000		☑
g100115	g100115		1.000		☑
k101	k101		0.005		☑
g10136	g10136		1.000		☑
g10151	g10151		1.000		☑
g101115	g101115		1.000		☑
k102	k102		0.005		☑
g10210	g10210		1.000		☑
g10251	g10251		1.000		☑
g102115	g102115		1.000		☑
k115	k115		0.500		☑
g11565	g11565		1.000		☑
g11566	g11566		1.000		☑
g115118	g115118		1.000		☑
k116	k116		0.500		☑
g11642	g11642		1.000		☑
g116118	g116118		1.000		☑
k1_0	k1’		$5.4 \cdot 10^{-5}$		⊟
k2_0	k2’		$-1.91 \cdot 10^{-4}$		⊟
k4_0	k4’		$-2.475 \cdot 10^{-5}$		⊟
k13_0	k13’		$-2.5 \cdot 10^{-6}$		⊟
k15_0	k15’		-10^{-5}		⊟
k32_0	k32’		$1.8 \cdot 10^{-7}$		⊟
k35_0	k35’		$1.8 \cdot 10^{-7}$		⊟
k36_0	k36’		$-9 \cdot 10^{-6}$		⊟
k38_0	k38’		$-1.925 \cdot 10^{-5}$		⊟
k46_0	k46’		$-5.4 \cdot 10^{-6}$		⊟
k47_0	k47’		$-5.4 \cdot 10^{-6}$		⊟
k48_0	k48’		$-5.4 \cdot 10^{-6}$		⊟

6 Function definitions

This is an overview of seven function definitions.

6.1 Function definition J3Sub

Name J3Sub

Arguments K, X1, G1, X2, G2, X3, G3

Mathematical Expression

$$K \cdot X1^{G1} \cdot X2^{G2} \cdot X3^{G3} \tag{1}$$

6.2 Function definition J1Sub

Name J1Sub

Arguments K, X, G

Mathematical Expression

$$K \cdot X^{G} \tag{2}$$

6.3 Function definition J2Sub

Name J2Sub

Arguments K, X1, G1, X2, G2

Mathematical Expression

$$K \cdot X1^{G1} \cdot X2^{G2} \tag{3}$$

6.4 Function definition J1Sub3Mod

Name J1Sub3Mod

Arguments K, X1, G1, X2, G2, X3, G3, X4, G4

Mathematical Expression

$$K \cdot X1^{G1} \cdot X2^{G2} \cdot X3^{G3} \cdot X4^{G4} \tag{4}$$

6.5 Function definition J2Sub1Mod

Name J2Sub1Mod

Arguments K, X1, G1, X2, G2, X3, G3

Mathematical Expression

$$K \cdot X1^{G1} \cdot X2^{G2} \cdot X3^{G3} \tag{5}$$

6.6 Function definition J1Sub1Mod

Name J1Sub1Mod

Arguments K, X1, G1, X2, G2

Mathematical Expression

$$\mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{6}$$

6.7 Function definition J3Sub1Mod

Name J3Sub1Mod

Arguments K, X1, G1, X2, G2, X3, G3, X4, G4

Mathematical Expression

$$\mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \cdot \mathrm{X4}^{\mathrm{G4}} \tag{7}$$

7 Rules

This is an overview of 13 rules.

7.1 Rule k1_0

Rule k1_0 is an assignment rule for parameter k1_0:

$$\mathrm{k1\_0} = 3 \cdot 10^{-4} \cdot (\mathrm{p18} \cdot [\mathrm{OH\_radical}] + \mathrm{p19} \cdot [\mathrm{H2O2}] + \mathrm{p110} \cdot [\mathrm{DA\_quinone}] + \mathrm{p186} \cdot [\mathrm{O2}]) \tag{8}$$

7.2 Rule k2_0

Rule k2_0 is an assignment rule for parameter k2_0:

$$\mathrm{k2\_0} = 10\hat{}\text{-}4 \cdot (\mathrm{i26} \cdot [\mathrm{Dopamine}] + \mathrm{p28} \cdot [\mathrm{OH\_radical}] + \mathrm{p29} \cdot [\mathrm{H2O2}] + \mathrm{p210} \cdot [\mathrm{DA\_quinone}] + \mathrm{p286} \cdot [\mathrm{O2}]) \tag{9}$$

7.3 Rule k4_0

Rule k4_0 is an assignment rule for parameter k4_0:

$$\mathrm{k4\_0} = 0.0090 \cdot (\mathrm{i41} \cdot [\mathrm{Alpha\_synuclein}] + \mathrm{i42} \cdot [\mathrm{Protofibril}] + \mathrm{i43} \cdot [\mathrm{Fibril}]) \tag{10}$$

7.4 Rule k13_0

Rule k13_0 is an assignment rule for parameter k13_0:

$$\mathrm{k13\_0} = 0.0010 \cdot (\mathrm{i131} \cdot [\mathrm{Alpha\_synuclein}] + \mathrm{i1310} \cdot [\mathrm{DA\_quinone}]) \tag{11}$$

7.5 Rule k15_0

Rule k15_0 is an assignment rule for parameter k15_0:

$$\mathrm{k15\_0} = 0.0020 \cdot \mathrm{i152} \cdot [\mathrm{Protofibril}] \tag{12}$$

7.6 Rule k32_0

Rule k32_0 is an assignment rule for parameter k32_0:

$$\mathrm{k32\_0} = 1.0E-5 \cdot (\mathrm{p328} \cdot [\mathrm{OH\_radical}] + \mathrm{p329} \cdot [\mathrm{H2O2}] + \mathrm{p3210} \cdot [\mathrm{DA\_quinone}] + \mathrm{p3286} \cdot [\mathrm{O2}]) \tag{13}$$

7.7 Rule k35_0

Rule k35_0 is an assignment rule for parameter k35_0:

$$\mathrm{k35\_0} = 1.0E-5 \cdot (\mathrm{p358} \cdot [\mathrm{OH\_radical}] + \mathrm{p359} \cdot [\mathrm{H2O2}] + \mathrm{p3510} \cdot [\mathrm{DA\_quinone}] + \mathrm{p3586} \cdot [\mathrm{O2}]) \tag{14}$$

7.8 Rule k36_0

Rule k36_0 is an assignment rule for parameter k36_0:

$$\mathrm{k36\_0} = 5 \cdot 10^{-4} \cdot (\mathrm{i368} \cdot [\mathrm{OH\_radical}] + \mathrm{i369} \cdot [\mathrm{H2O2}] + \mathrm{i3610} \cdot [\mathrm{DA\_quinone}] + \mathrm{i3686} \cdot [\mathrm{O2}]) \tag{15}$$

7.9 Rule k38_0

Rule k38_0 is an assignment rule for parameter k38_0:

$$\mathrm{k38\_0} = 0.0070 \cdot (\mathrm{i381} \cdot [\mathrm{Alpha\_synuclein}] + \mathrm{i382} \cdot [\mathrm{Protofibril}] + \mathrm{i383} \cdot [\mathrm{Fibril}]) \tag{16}$$

7.10 Rule k46_0

Rule k46_0 is an assignment rule for parameter k46_0:

$$\mathrm{k46\_0} = 3 \cdot 10^{-4} \cdot (\mathrm{i468} \cdot [\mathrm{OH\_radical}] + \mathrm{i469} \cdot [\mathrm{H2O2}] + \mathrm{i4610} \cdot [\mathrm{DA\_quinone}] + \mathrm{i4686} \cdot [\mathrm{O2}]) \tag{17}$$

7.11 Rule k47_0

Rule k47_0 is an assignment rule for parameter k47_0:

$$\mathrm{k47\_0} = 3 \cdot 10^{-4} \cdot (\mathrm{i478} \cdot [\mathrm{OH\_radical}] + \mathrm{i479} \cdot [\mathrm{H2O2}] + \mathrm{i4710} \cdot [\mathrm{DA\_quinone}] + \mathrm{i4786} \cdot [\mathrm{O2}]) \tag{18}$$

7.12 Rule k48_0

Rule k48_0 is an assignment rule for parameter k48_0:

$$\mathrm{k48\_0} = 3 \cdot 10^{-4} \cdot (\mathrm{i488} \cdot [\mathrm{OH\_radical}] + \mathrm{i489} \cdot [\mathrm{H2O2}] + \mathrm{i4810} \cdot [\mathrm{DA\_quinone}] + \mathrm{i4886} \cdot [\mathrm{O2}]) \tag{19}$$

7.13 Rule Fe2

Rule Fe2 is a rate rule for species Fe2:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fe2} = \mathrm{J21} - \mathrm{J20} + 0.01 \tag{20}$$

8 Reactions

This model contains 58 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	J1	J1	Alpha_synuclein $\xrightarrow{\text{Alpha\_synuclein, Alpha\_synuclein, Alpha\_synuclein, Alpha\_synuclein}}$	
2	J2	J2	Protofibril $\xrightarrow{\text{Protofibril, Protofibril, Protofibril, Protofibril, Protofibril, Protofibril, Protofi}}$	
3	J3	J3	Fibril + Parkin_synphilin_1_ub $\xrightarrow{\text{Fibril, Parkin\_synphilin\_1\_ub, Fibril, Parkin\_synphilin\_1}}$	
4	J4	J4	Parkin_sub_ub4 $\xrightarrow{\text{Proteasome\_0, ATP, UCH\_L1, Parkin\_sub\_ub4, Proteasome\_0, ATP, U}}$ Fragments + 4 Ubiquitin	
5	J6	J6	Ubiquitin + E1 $\xrightarrow{\text{ATP, Ubiquitin, E1, ATP, Ubiquitin, E1, ATP, Ubiquitin, E1, ATP, Ubi}}$	
6	J7	J7	Ub_E1 + UbcH8 $\xrightarrow{\text{ATP, Ub\_E1, UbcH8, ATP, Ub\_E1, UbcH8, ATP, Ub\_E1, UbcH8, AT}}$ UbcH8_Ub	
7	J8	J8	Parkin + Substrate $\xrightarrow{\text{Parkin, Substrate, Parkin, Substrate, Parkin, Substrate, Parkin, Subst}}$	
8	J9	J9	Parkin + Synphilin_1 $\xrightarrow{\text{Parkin, Synphilin\_1, Parkin, Synphilin\_1, Parkin, Synphilin\_1, Pa}}$	
9	J10	J10	Parkin_synphilin_1 + UbcH13_Uev1a_ub $\xrightarrow{\text{Parkin\_synphilin\_1, UbcH13\_Uev1a\_ub, Parkin\_synphilin\_1, UbcH}}$ Parkin_synphilin_1 + UbcH13_Uev1a	
10	J11	J11	Parkin_sub + UbcH8ub4 $\xrightarrow{\text{Parkin\_sub, UbcH8ub4, Parkin\_sub, UbcH8ub4, Parkin\_sub, U}}$ UbcH8	
11	J13	J13	L_Tyr + O2_0 $\xrightarrow{\text{TH, L\_Tyr, O2\_0, TH, L\_Tyr, O2\_0, TH, L\_Tyr, O2\_0, TH, L\_Tyr, O2\_0,}}$	

№	Id	Name	Reaction Equation	SBO
12	J14	J14	$\text{L\_Dopa} \xrightarrow{\text{DDC, L\_Dopa, DDC, L\_Dopa, DDC, L\_Dopa, DDC, L\_Dopa, DDC, L\_Dopa,}} \text{CO2}$	
13	J15	J15	$\text{Dopamine} + \text{Vesicle\_0} \xrightarrow{\text{VMAT2, Dopamine, Vesicle\_0, VMAT2, Dopamine, Vesicle\_0,}}$	
14	J16	J16	$\text{Bioamines} + \text{Vesicle\_0} \xrightarrow{\text{Bioamines, Vesicle\_0, Bioamines, Vesicle\_0, Bioamines, Vesicle}}$	
15	J17	J17	$\text{Neurotoxins} + \text{Vesicle\_0} \xrightarrow{\text{Neurotoxins, Vesicle\_0, Neurotoxins, Vesicle\_0, Neurotoxins,}}$	
16	J18	J18	$\text{Dopamine} + \text{O2\_0} \xrightarrow{\text{Dopamine, O2\_0, Dopamine, O2\_0, Dopamine, O2\_0, Dopamine, O}} \text{O2}$	
17	J19	J19	$\text{Dopamine} + \text{O2\_0} + \text{H2O} \xrightarrow{\text{MAO, Dopamine, O2\_0, H2O, MAO, Dopamine, O2\_0, H2O, MAO, Dopamine,}} \text{DOPAL} + \text{H2O2}$	
18	J20	J20	$\text{H2O2} + \text{Fe2} \xrightarrow{\text{H2O2, Fe2, H2O2, Fe2, H2O2, Fe2, H2O2, Fe2, H2O2, Fe2, H2O2, Fe2,}} \text{OH\_radical} + \text{OH}$	
19	J21	J21	$\text{Fe3} \xrightarrow{\text{Fe3, Fe3, Fe3, Fe3, Fe3, Fe3, Fe3, Fe3, Fe3}} \text{Fe2}$	
20	J22	J22	$\text{H2O2} \xrightarrow{\text{Catalase, H2O2, Catalase, H2O2, Catalase, H2O2, Catalase, H2O2, Catalase, H}} \text{O2\_0}$	
21	J23	J23	$\text{H2O2} + \text{GSH} \xrightarrow{\text{Gluta\_per, H2O2, GSH, Gluta\_per, H2O2, GSH, Gluta\_per, H2O2, GSH}} \text{GSSG}$	
22	J24	J24	$\text{GSSG} \xrightarrow{\text{Gluta\_red, GSSG, Gluta\_red, GSSG, Gluta\_red, GSSG, Gluta\_red, GSSG, Gluta}}$	
23	J25	J25	$\text{DOPAL} + \text{NAD} \xrightarrow{\text{ALDH, DOPAL, NAD, ALDH, DOPAL, NAD, ALDH, DOPAL, NAD}} \text{NADH}$	
24	J26f	J26f	$\text{Ub\_E1} + \text{UbcH8\_Ub} \xrightarrow{\text{ATP, Ub\_E1, UbcH8\_Ub, ATP, Ub\_E1, UbcH8\_Ub, ATP, Ub\_E1,}} \text{UbcH8ub2}$	

№	Id	Name	Reaction Equation	SBO
25	J26r	J26r	UbcH8ub2 $\xrightarrow{\text{UCH\_L1, UbcH8ub2, UCH\_L1, UbcH8ub2, UCH\_L1, UbcH8ub2, UCH\_L}}$ 2 Ubiquitin	
26	J27f	J27f	Ub_E1 + UbcH8ub2 $\xrightarrow{\text{ATP, Ub\_E1, UbcH8ub2, ATP, Ub\_E1, UbcH8ub2, ATP, Ub\_E1,}}$ UbcH8ub3	
27	J27r	J27r	UbcH8ub3 $\xrightarrow{\text{UCH\_L1, UbcH8ub3, UCH\_L1, UbcH8ub3, UCH\_L1, UbcH8ub3, UCH\_L}}$ 3 Ubiquitin	
28	J28f	J28f	Ub_E1 + UbcH8ub3 $\xrightarrow{\text{ATP, Ub\_E1, UbcH8ub3, ATP, Ub\_E1, UbcH8ub3, ATP, Ub\_E1,}}$ UbcH8ub4	
29	J28r	J28r	UbcH8ub4 $\xrightarrow{\text{UCH\_L1, UbcH8ub4, UCH\_L1, UbcH8ub4, UCH\_L1, UbcH8ub4, UCH\_L}}$ 4 Ubiquitin	
30	J29	J29	Ub_E1 + UbcH13_Uev1a $\xrightarrow{\text{ATP, Ub\_E1, UbcH13\_Uev1a, ATP, Ub\_E1, UbcH13\_Uev1a,}}$ UbcH13_Uev1a_ub	
31	J30	J30	Alpha_synuclein + UCH_L1 $\xrightarrow{\text{Alpha\_synuclein, UCH\_L1, Alpha\_synuclein, UCH\_L1, Alpha\_synuclein, UC}}$	
32	J31	J31	UbcH13_Uev1a_ub + asyn_UCH_L1 $\xrightarrow{\text{UbcH13\_Uev1a\_ub, asyn\_UCH\_L1, UbcH13\_Uev1a\_ub, asyn\_UCH\_L1,}}$ UCH_L1 + asyn_ub	
33	J32	J32	Alpha_synuclein + asyn_ub $\xrightarrow{\text{Alpha\_synuclein, asyn\_ub, Alpha\_synuclein, asyn\_ub, Alpha\_synuclein, asyn\_u}}$	
34	J33	J33	Protofibril + UCH_L1 $\xrightarrow{\text{Protofibril, UCH\_L1, Protofibril, UCH\_L1, Protofibril, UCH\_L1,}}$	
35	J34	J34	UbcH13_Uev1a_ub + Protofibril_UCH_L1 $\xrightarrow{\text{UbcH13\_Uev1a\_ub, Protofibril\_UCH\_L1, UbcH13\_Uev1a\_ub, Prot}}$ UCH_L1 + Protofibril_Ub	
36	J35	J35	Protofibril + Protofibril_Ub $\xrightarrow{\text{Protofibril, Protofibril\_Ub, Protofibril, Protofibril\_Ub, Proto}}$	

№	Id	Name	Reaction Equation	SBO
37	J36	J36	Autophagosome_0 $\xrightarrow{\text{Lysosome\_0, Autophagosome\_0, Lysosome\_0, Autophagosome\_0, L}}$	
38	J37	J37	UbcH8ub4 + asyn_UCH_L1 $\xrightarrow{\text{UbcH8ub4, asyn\_UCH\_L1, UbcH8ub4, asyn\_UCH\_L1, Ub}}$ UbcH8	
39	J38	J38	UCH_L1_asyn_ub4 $\xrightarrow{\text{Proteasome\_0, ATP, UCH\_L1, UCH\_L1\_asyn\_ub4, Proteasome\_0, A}}$ UCH_L1 + 4 Ubiquitin	
40	J43	J43	Alpha_synuclein + Hsc70 $\xrightarrow{\text{Alpha\_synuclein, Hsc70, Alpha\_synuclein, Hsc70, Alpha\_synuclein, Hsc70, Alp}}$	
41	J44	J44	Protofibril + Hsc70 $\xrightarrow{\text{Protofibril, Hsc70, Protofibril, Hsc70, Protofibril, Hsc70, Protofibri}}$	
42	J45	J45	Fibril + Hsc70 $\xrightarrow{\text{Fibril, Hsc70, Fibril, Hsc70, Fibril, Hsc70, Fibril, Hsc70, Fibril, Hsc70,}}$	
43	J46	J46	Hsc70_asyn $\xrightarrow{\text{Lysosome\_0, Hsc70\_asyn, Lysosome\_0, Hsc70\_asyn, Lysosome\_0, Hsc70\_}}$ Fragments	
44	J47	J47	Hsc70_Protofibril $\xrightarrow{\text{Lysosome\_0, Hsc70\_Protofibril, Lysosome\_0, Hsc70\_Protofibril, Lys}}$ Fragments	
45	J48	J48	Hsc70_fibril $\xrightarrow{\text{Lysosome\_0, Hsc70\_fibril, Lysosome\_0, Hsc70\_fibril, Lysosome\_0, Hsc70}}$ Fragments	
46	J50	J50	Alpha_synuclein + Preautophagosome_membrane $\xrightarrow{\text{Alpha\_synuclein, Preautophagosome\_membrane, Alpha}}$	
47	J51	J51	Protofibril + Preautophagosome_membrane $\xrightarrow{\text{Protofibril, Preautophagosome\_membrane,}}$	
48	J52	J52	Fibril + Preautophagosome_membrane $\xrightarrow{\text{Fibril, Preautophagosome\_membrane, Fibril, Pr}}$	
49	J53	J53	Lewy_body + Preautophagosome_membrane $\xrightarrow{\text{Lewy\_body, Preautophagosome\_membran}}$	
50	J54	J54	DA_quinone + Parkin $\xrightarrow{\text{DA\_quinone, Parkin, DA\_quinone, Parkin, DA\_quinone, Parkin,}}$	

№	Id	Name	Reaction Equation	SBO
51	J55	J55	Dopamine + O2 → DA_quinone	Dopamine, O2, Dopamine, O2, Dopamine, O2, Dopamine, O2, Dopar
52	J56	J56	O2 → O2_0	SOD, O2, SOD, O2, SOD, O2, SOD, O2, SOD, O2, SOD, O2, SOD, O2, SOD, O
53	J57	J57	DA_quinone + GSH →	DA_quinone, GSH, DA_quinone, GSH, DA_quinone, GSH, DA_qu
54	J100	J100	L_Dopa + O2_0 + Cysteine → H2O2 + CO2	L_Dopa, O2_0, Cysteine, L_Dopa, O2_0, Cysteine, L_Dopa, O2_0, Cysteine,
55	J101	J101	L_Tyr + O2_0 + Cysteine → H2O2 + CO2	L_Tyr, O2_0, Cysteine, L_Tyr, O2_0, Cysteine, L_Tyr, O2_0, C
56	J102	J102	DA_quinone + O2_0 + Cysteine → CO2	DA_quinone, O2_0, Cysteine, DA_quinone, O2_0, Cysteine, DA_quinone, O2
57	J115	J115	Fe3 + Neuromelanin →	Fe3, Neuromelanin, Fe3, Neuromelanin, Fe3, Neuromelanin, Fe3
58	J116	J116	Neuromelanin + Neurotoxins →	Neuromelanin, Neurotoxins, Neuromelanin, Neurotoxins

8.1 Reaction J1

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

Name J1

Notes Protofibril aggregation

Reaction equation

$$\text{Alpha\_synuclein} \xrightarrow{\text{Alpha\_synuclein, Alpha\_synuclein, Alpha\_synuclein, Alpha\_synuclein, Alpha\_synuclein, Alpha\_sy}} \tag{21}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
Alpha_synuclein	Alpha_synuclein	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
Alpha_synuclein	Alpha_synuclein	
Alpha_synuclein	Alpha_synuclein	
Alpha_synuclein	Alpha_synuclein	
Alpha_synuclein	Alpha_synuclein	
Alpha_synuclein	Alpha_synuclein	
Alpha_synuclein	Alpha_synuclein	
Alpha_synuclein	Alpha_synuclein	
Alpha_synuclein	Alpha_synuclein	
Alpha_synuclein	Alpha_synuclein	

Product

Table 8: Properties of each product.

Id	Name	SBO
Protofibril	Protofibril	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J1Sub}\left(\mathrm{k1}, [\mathrm{Alpha\_synuclein}], \mathrm{g11}\right) \tag{22}$$

$$\mathrm{J1Sub}\left(\mathrm{K}, \mathrm{X}, \mathrm{G}\right) = \mathrm{K} \cdot \mathrm{X}^{\mathrm{G}} \tag{23}$$

$$\mathrm{J1Sub}\left(\mathrm{K}, \mathrm{X}, \mathrm{G}\right) = \mathrm{K} \cdot \mathrm{X}^{\mathrm{G}} \tag{24}$$

8.2 Reaction J2

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

Name J2

Notes `Fibril aggregation`

Reaction equation

$$\mathrm{Protofibril} \xrightarrow{\mathrm{Protofibril,\ Protofibril,\ Protofibril,\ Protofibril,\ Protofibril,\ Protofibril,\ Protofibril,\ Protofibril,\ Protofibril}} \mathrm{F} \tag{25}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
`Protofibril`	Protofibril	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
`Protofibril`	Protofibril	
`Protofibril`	Protofibril	
`Protofibril`	Protofibril	
`Protofibril`	Protofibril	
`Protofibril`	Protofibril	
`Protofibril`	Protofibril	
`Protofibril`	Protofibril	

Id	Name	SBO
Protofibril	Protofibril	
Protofibril	Protofibril	

Product

Table 11: Properties of each product.

Id	Name	SBO
Fibril	Fibril	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}\left(\text{Neuronal\_cytosol}\right) \cdot \text{J1Sub}\left(\text{k2}, [\text{Protofibril}], \text{g22}\right) \tag{26}$$

$$\text{J1Sub}\left(\text{K}, \text{X}, \text{G}\right) = \text{K} \cdot \text{X}^{\text{G}} \tag{27}$$

$$\text{J1Sub}\left(\text{K}, \text{X}, \text{G}\right) = \text{K} \cdot \text{X}^{\text{G}} \tag{28}$$

8.3 Reaction J3

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J3

Notes Lewy Body formation

Reaction equation

$$\text{Fibril} + \text{Parkin\_synphilin\_1\_ub} \xrightarrow{\text{Fibril, Parkin\_synphilin\_1\_ub, Fibril, Parkin\_synphilin\_1\_ub, Fibril, Parkin\_synphilin\_} \quad (29)$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
Fibril	Fibril	
Parkin_synphilin_1_ub	Parkin-synphilin-1-ub	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
Fibril	Fibril	
Parkin_synphilin_1_ub	Parkin-synphilin-1-ub	
Fibril	Fibril	
Parkin_synphilin_1_ub	Parkin-synphilin-1-ub	
Fibril	Fibril	
Parkin_synphilin_1_ub	Parkin-synphilin-1-ub	
Fibril	Fibril	
Parkin_synphilin_1_ub	Parkin-synphilin-1-ub	
Fibril	Fibril	
Parkin_synphilin_1_ub	Parkin-synphilin-1-ub	
Fibril	Fibril	
Parkin_synphilin_1_ub	Parkin-synphilin-1-ub	
Fibril	Fibril	
Parkin_synphilin_1_ub	Parkin-synphilin-1-ub	
Fibril	Fibril	
Parkin_synphilin_1_ub	Parkin-synphilin-1-ub	
Fibril	Fibril	
Parkin_synphilin_1_ub	Parkin-synphilin-1-ub	

Product

Table 14: Properties of each product.

Id	Name	SBO
Lewy_body	Lewy_body	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k3}, [\mathrm{Fibril}], \mathrm{g23}, [\mathrm{Parkin\_synphilin\_1\_ub}], \mathrm{g326}\right) \quad (30)$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (31)$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (32)$$

8.4 Reaction J4

This is an irreversible reaction of one reactant forming three products influenced by 39 modifiers.

Name J4

Notes Proteasome Degradation of parkin-sub-ub4

Reaction equation

$$\text{Parkin\_sub\_ub4} \xrightarrow{\text{Proteasome\_0, ATP, UCH\_L1, Parkin\_sub\_ub4, Proteasome\_0, ATP, UCH\_L1, Parkin\_sub\_ub4, Prot}} \quad (33)$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
Parkin_sub_ub4	Parkin-sub-ub4	

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
Parkin_sub_ub4	Parkin-sub-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
Parkin_sub_ub4	Parkin-sub-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
Parkin_sub_ub4	Parkin-sub-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
Parkin_sub_ub4	Parkin-sub-ub4	
Proteasome_0	Proteasome	
ATP	ATP	

Id	Name	SBO
UCH_L1	UCH-L1	
Parkin_sub_ub4	Parkin-sub-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
Parkin_sub_ub4	Parkin-sub-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
Parkin_sub_ub4	Parkin-sub-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
Parkin_sub_ub4	Parkin-sub-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
Parkin_sub_ub4	Parkin-sub-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	

Products

Table 17: Properties of each product.

Id	Name	SBO
Parkin	Parkin	
Fragments	Fragments	
Ubiquitin	Ubiquitin	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J1Sub3Mod}\left(\mathrm{k4}, [\mathrm{Parkin\_sub\_ub4}], \mathrm{g427}, [\mathrm{Proteasome\_0}], \mathrm{g412}, [\mathrm{ATP}], \mathrm{g415}, [\mathrm{UCH\_L1}], \mathrm{g430}\right) \quad (34)$$

$$\mathrm{J1Sub3Mod}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}, \mathrm{X4}, \mathrm{G4}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \cdot \mathrm{X4}^{\mathrm{G4}} \quad (35)$$

$$\mathrm{J1Sub3Mod}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}, \mathrm{X4}, \mathrm{G4}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \cdot \mathrm{X4}^{\mathrm{G4}} \quad (36)$$

8.5 Reaction J6

This is an irreversible reaction of two reactants forming one product influenced by 28 modifiers.

Name J6

Notes `Ubiquitin Activation`

Reaction equation

$$\text{Ubiquitin} + \text{E1} \xrightarrow{\text{ATP, Ubiquitin, E1, ATP, Ubiquitin, E1, ATP, Ubiquitin, E1, ATP, Ubiquitin, E1, ATP, Ubiquitin,}} \quad (37)$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
`Ubiquitin`	Ubiquitin	
`E1`	E1	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
`ATP`	ATP	
`Ubiquitin`	Ubiquitin	
`E1`	E1	
`ATP`	ATP	
`Ubiquitin`	Ubiquitin	
`E1`	E1	
`ATP`	ATP	
`Ubiquitin`	Ubiquitin	
`E1`	E1	
`ATP`	ATP	
`Ubiquitin`	Ubiquitin	
`E1`	E1	
`ATP`	ATP	
`Ubiquitin`	Ubiquitin	
`E1`	E1	
`ATP`	ATP	
`Ubiquitin`	Ubiquitin	

Id	Name	SBO
E1	E1	
ATP	ATP	
Ubiquitin	Ubiquitin	
E1	E1	
ATP	ATP	
Ubiquitin	Ubiquitin	
E1	E1	
ATP	ATP	
Ubiquitin	Ubiquitin	
E1	E1	
ATP	ATP	

Product

Table 20: Properties of each product.

Id	Name	SBO
Ub_E1	Ub-E1	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J2Sub1Mod}\,(\text{k6}, [\text{Ubiquitin}], \text{g613}, [\text{E1}], \text{g614}, [\text{ATP}], \text{g615}) \quad (38)$$

$$\text{J2Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}, \text{X3}, \text{G3}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \cdot \text{X3}^{\text{G3}} \quad (39)$$

$$\text{J2Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}, \text{X3}, \text{G3}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \cdot \text{X3}^{\text{G3}} \quad (40)$$

8.6 Reaction J7

This is an irreversible reaction of two reactants forming two products influenced by 28 modifiers.

Name J7

Notes Ubiquitin Conjugation

Reaction equation

$$\text{Ub\_E1} + \text{UbcH8} \xrightarrow{\text{ATP, Ub\_E1, UbcH8, ATP, Ub\_E1, UbcH8, ATP, Ub\_E1, UbcH8, ATP, Ub\_E1, UbcH8, ATP, Ub\_} \quad (41)$$

Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
Ub_E1	Ub-E1	
UbcH8	UbcH8	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8	UbcH8	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8	UbcH8	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8	UbcH8	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8	UbcH8	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8	UbcH8	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8	UbcH8	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8	UbcH8	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8	UbcH8	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8	UbcH8	
ATP	ATP	

Products

Table 23: Properties of each product.

Id	Name	SBO
E1	E1	
UbcH8_Ub	UbcH8-Ub	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{Neuronal\_cytosol}) \cdot \mathrm{J2Sub1Mod}\,(\mathrm{k7}, [\mathrm{Ub\_E1}], \mathrm{g716}, [\mathrm{UbcH8}], \mathrm{g717}, [\mathrm{ATP}], \mathrm{g715}) \quad (42)$$

$$\mathrm{J2Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \quad (43)$$

$$\mathrm{J2Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \quad (44)$$

8.7 Reaction J8

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J8

Notes Substrate ligation

Reaction equation

$$\mathrm{Parkin} + \mathrm{Substrate} \xrightarrow{\mathrm{Parkin,\ Substrate,\ Parkin,\ Substrate,\ Parkin,\ Substrate,\ Parkin,\ Substrate,\ Parkin,\ Substrate,\ Parki}} \quad (45)$$

Reactants

Table 24: Properties of each reactant.

Id	Name	SBO
Parkin	Parkin	
Substrate	Substrate	

Modifiers

Table 25: Properties of each modifier.

Id	Name	SBO
Parkin	Parkin	
Substrate	Substrate	
Parkin	Parkin	
Substrate	Substrate	
Parkin	Parkin	
Substrate	Substrate	
Parkin	Parkin	
Substrate	Substrate	
Parkin	Parkin	
Substrate	Substrate	
Parkin	Parkin	
Substrate	Substrate	
Parkin	Parkin	
Substrate	Substrate	
Parkin	Parkin	
Substrate	Substrate	
Parkin	Parkin	
Substrate	Substrate	

Product

Table 26: Properties of each product.

Id	Name	SBO
Parkin_sub	Parkin-sub	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k8}, [\mathrm{Parkin}], \mathrm{g819}, [\mathrm{Substrate}], \mathrm{g821}\right) \tag{46}$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{47}$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{48}$$

8.8 Reaction J9

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J9

Notes Synphilin-1 ligation

Reaction equation

$$\text{Parkin} + \text{Synphilin\_1} \xrightarrow{\text{Parkin, Synphilin\_1, Parkin, Synphilin\_1, Parkin, Synphilin\_1, Parkin, Synphilin\_1, Parkin, Sy}} \tag{49}$$

Reactants

Table 27: Properties of each reactant.

Id	Name	SBO
Parkin	Parkin	
Synphilin_1	Synphilin-1	

Modifiers

Table 28: Properties of each modifier.

Id	Name	SBO
Parkin	Parkin	
Synphilin_1	Synphilin-1	
Parkin	Parkin	
Synphilin_1	Synphilin-1	
Parkin	Parkin	
Synphilin_1	Synphilin-1	
Parkin	Parkin	
Synphilin_1	Synphilin-1	
Parkin	Parkin	
Synphilin_1	Synphilin-1	
Parkin	Parkin	
Synphilin_1	Synphilin-1	
Parkin	Parkin	
Synphilin_1	Synphilin-1	
Parkin	Parkin	
Synphilin_1	Synphilin-1	
Parkin	Parkin	

Id	Name	SBO
Synphilin_1	Synphilin-1	

Product

Table 29: Properties of each product.

Id	Name	SBO
Parkin_synphilin_1	Parkin-synphilin-1	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J2Sub}\,(\text{k9}, [\text{Parkin}], \text{g919}, [\text{Synphilin\_1}], \text{g920}) \tag{50}$$

$$\text{J2Sub}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \tag{51}$$

$$\text{J2Sub}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \tag{52}$$

8.9 Reaction J10

This is an irreversible reaction of two reactants forming two products influenced by 18 modifiers.

Name J10

Notes K63 Synphilin-1 Ubiquitination

Reaction equation

$$\text{Parkin\_synphilin\_1} + \text{UbcH13\_Uev1a\_ub} \xrightarrow{\text{Parkin\_synphilin\_1, UbcH13\_Uev1a\_ub, Parkin\_synphilin\_1, UbcH13\_Uev}} \tag{53}$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
Parkin_synphilin_1	Parkin-synphilin-1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
Parkin_synphilin_1	Parkin-synphilin-1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Parkin_synphilin_1	Parkin-synphilin-1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Parkin_synphilin_1	Parkin-synphilin-1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Parkin_synphilin_1	Parkin-synphilin-1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Parkin_synphilin_1	Parkin-synphilin-1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Parkin_synphilin_1	Parkin-synphilin-1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Parkin_synphilin_1	Parkin-synphilin-1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Parkin_synphilin_1	Parkin-synphilin-1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Parkin_synphilin_1	Parkin-synphilin-1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	

Products

Table 32: Properties of each product.

Id	Name	SBO
Parkin_synphilin_1_ub	Parkin-synphilin-1-ub	
UbcH13_Uev1a	UbcH13/Uev1a	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k10}, [\mathrm{Parkin\_synphilin\_1}], \mathrm{g1025}, [\mathrm{UbcH13\_Uev1a\_ub}], \mathrm{g1072}\right) \quad (54)$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (55)$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (56)$$

8.10 Reaction J11

This is an irreversible reaction of two reactants forming two products influenced by 18 modifiers.

Name J11

Notes K48 Substrate Ubiquitination

Reaction equation

$$\text{Parkin\_sub} + \text{UbcH8ub4} \xrightarrow{\text{Parkin\_sub, UbcH8ub4, Parkin\_sub, UbcH8ub4, Parkin\_sub, UbcH8ub4, Parkin\_sub, UbcH}} \quad (57)$$

Reactants

Table 33: Properties of each reactant.

Id	Name	SBO
Parkin_sub	Parkin-sub	
UbcH8ub4	UbcH8ub4	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
Parkin_sub	Parkin-sub	
UbcH8ub4	UbcH8ub4	
Parkin_sub	Parkin-sub	
UbcH8ub4	UbcH8ub4	
Parkin_sub	Parkin-sub	
UbcH8ub4	UbcH8ub4	
Parkin_sub	Parkin-sub	
UbcH8ub4	UbcH8ub4	
Parkin_sub	Parkin-sub	
UbcH8ub4	UbcH8ub4	
Parkin_sub	Parkin-sub	
UbcH8ub4	UbcH8ub4	
Parkin_sub	Parkin-sub	
UbcH8ub4	UbcH8ub4	
Parkin_sub	Parkin-sub	
UbcH8ub4	UbcH8ub4	
Parkin_sub	Parkin-sub	

Id	Name	SBO
UbcH8ub4	UbcH8ub4	

Products

Table 35: Properties of each product.

Id	Name	SBO
Parkin_sub_ub4	Parkin-sub-ub4	
UbcH8	UbcH8	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k11}, [\mathrm{Parkin\_sub}], \mathrm{g1124}, [\mathrm{UbcH8ub4}], \mathrm{g1170}\right) \quad (58)$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (59)$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (60)$$

8.11 Reaction J13

This is an irreversible reaction of two reactants forming one product influenced by 28 modifiers.

Name J13

Notes L-Dopa formation

Reaction equation

$$\mathrm{L\_Tyr} + \mathrm{O2\_0} \xrightarrow{\mathrm{TH},\ \mathrm{L\_Tyr},\ \mathrm{O2\_0},\ \mathrm{TH},\ \mathrm{L\_Tyr},\ \mathrm{O2\_0},\ \mathrm{TH},\ \mathrm{L\_Tyr},\ \mathrm{O2\_0},\ \mathrm{TH},\ \mathrm{L\_Tyr},\ \mathrm{O2\_0},\ \mathrm{TH},\ \mathrm{L\_Tyr},\ \mathrm{O2\_0},\ \mathrm{TH},\ \mathrm{L\_Tyr}} \quad (61)$$

Reactants

Table 36: Properties of each reactant.

Id	Name	SBO
L_Tyr	L-Tyr	
O2_0	O2	

Modifiers

Table 37: Properties of each modifier.

Id	Name	SBO
TH	TH	
L_Tyr	L-Tyr	
O2_0	O2	
TH	TH	
L_Tyr	L-Tyr	
O2_0	O2	
TH	TH	
L_Tyr	L-Tyr	
O2_0	O2	
TH	TH	
L_Tyr	L-Tyr	
O2_0	O2	
TH	TH	
L_Tyr	L-Tyr	
O2_0	O2	
TH	TH	
L_Tyr	L-Tyr	
O2_0	O2	
TH	TH	
L_Tyr	L-Tyr	
O2_0	O2	
TH	TH	
L_Tyr	L-Tyr	
O2_0	O2	
TH	TH	
L_Tyr	L-Tyr	
O2_0	O2	
TH	TH	

Product

Table 38: Properties of each product.

Id	Name	SBO
L_Dopa	L-Dopa	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{Neuronal\_cytosol}) \cdot \mathrm{J2Sub1Mod}\,(\mathrm{k13}, [\mathrm{L\_Tyr}], \mathrm{g1336}, [\mathrm{O2\_0}], \mathrm{g1351}, [\mathrm{TH}], \mathrm{g1335}) \tag{62}$$

$$\mathrm{J2Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \tag{63}$$

$$\mathrm{J2Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \tag{64}$$

8.12 Reaction J14

This is an irreversible reaction of one reactant forming two products influenced by 19 modifiers.

Name J14

Notes Dopamine formation

Reaction equation

$$\mathrm{L\_Dopa} \xrightarrow{\mathrm{DDC},\ \mathrm{L\_Dopa},\ \mathrm{DDC},\ \mathrm{L\_Dopa},\ \mathrm{DDC},\ \mathrm{L\_Dopa},\ \mathrm{DDC},\ \mathrm{L\_Dopa},\ \mathrm{DDC},\ \mathrm{L\_Dopa},\ \mathrm{DDC},\ \mathrm{L\_Dopa},\ \mathrm{DDC},\ \mathrm{L\_Dop}} \tag{65}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
L_Dopa	L-Dopa	

Modifiers

Table 40: Properties of each modifier.

Id	Name	SBO
DDC	DDC	
L_Dopa	L-Dopa	
DDC	DDC	
L_Dopa	L-Dopa	
DDC	DDC	
L_Dopa	L-Dopa	

Id	Name	SBO
DDC	DDC	
L_Dopa	L-Dopa	
DDC	DDC	
L_Dopa	L-Dopa	
DDC	DDC	
L_Dopa	L-Dopa	
DDC	DDC	
L_Dopa	L-Dopa	
DDC	DDC	
L_Dopa	L-Dopa	
DDC	DDC	
L_Dopa	L-Dopa	
DDC	DDC	

Products

Table 41: Properties of each product.

Id	Name	SBO
Dopamine	Dopamine	
CO2	CO2	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J1Sub1Mod}\,(\text{k14}, [\text{L\_Dopa}], \text{g1437}, [\text{DDC}], \text{g1467}) \quad (66)$$

$$\text{J1Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (67)$$

$$\text{J1Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (68)$$

8.13 Reaction J15

This is an irreversible reaction of two reactants forming one product influenced by 28 modifiers.

Name J15

Notes Dopamine vesicle packaging

Reaction equation

$$\text{Dopamine} + \text{Vesicle\_0} \xrightarrow{\text{VMAT2, Dopamine, Vesicle\_0, VMAT2, Dopamine, Vesicle\_0, VMAT2, Dopamine, Vesicle}} \quad (69)$$

Reactants

Table 42: Properties of each reactant.

Id	Name	SBO
Dopamine	Dopamine	
Vesicle_0	Vesicle	

Modifiers

Table 43: Properties of each modifier.

Id	Name	SBO
VMAT2	VMAT2	
Dopamine	Dopamine	
Vesicle_0	Vesicle	
VMAT2	VMAT2	
Dopamine	Dopamine	
Vesicle_0	Vesicle	
VMAT2	VMAT2	
Dopamine	Dopamine	
Vesicle_0	Vesicle	
VMAT2	VMAT2	
Dopamine	Dopamine	
Vesicle_0	Vesicle	
VMAT2	VMAT2	
Dopamine	Dopamine	
Vesicle_0	Vesicle	
VMAT2	VMAT2	
Dopamine	Dopamine	
Vesicle_0	Vesicle	
VMAT2	VMAT2	
Dopamine	Dopamine	
Vesicle_0	Vesicle	
VMAT2	VMAT2	
Dopamine	Dopamine	
Vesicle_0	Vesicle	

Id	Name	SBO
VMAT2	VMAT2	
Dopamine	Dopamine	
Vesicle_0	Vesicle	
VMAT2	VMAT2	

Product

Table 44: Properties of each product.

Id	Name	SBO
V_DA	V-DA	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{J2Sub1Mod}\left(\text{k15}, [\text{Dopamine}], \text{g156}, [\text{Vesicle\_0}], \text{g1544}, [\text{VMAT2}], \text{g1545}\right) \quad (70)$$

$$\text{J2Sub1Mod}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}, \text{X3}, \text{G3}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \cdot \text{X3}^{\text{G3}} \quad (71)$$

8.14 Reaction J16

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J16

Notes Bioamine vesicle packaging

Reaction equation

$$\text{Bioamines} + \text{Vesicle\_0} \xrightarrow{\text{Bioamines, Vesicle\_0, Bioamines, Vesicle\_0, Bioamines, Vesicle\_0, Bioamines, Vesicle\_0, Bi}} \quad (72)$$

Reactants

Table 45: Properties of each reactant.

Id	Name	SBO
Bioamines	Bioamines	
Vesicle_0	Vesicle	

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
Bioamines	Bioamines	
Vesicle_0	Vesicle	
Bioamines	Bioamines	
Vesicle_0	Vesicle	
Bioamines	Bioamines	
Vesicle_0	Vesicle	
Bioamines	Bioamines	
Vesicle_0	Vesicle	
Bioamines	Bioamines	
Vesicle_0	Vesicle	
Bioamines	Bioamines	
Vesicle_0	Vesicle	
Bioamines	Bioamines	
Vesicle_0	Vesicle	
Bioamines	Bioamines	
Vesicle_0	Vesicle	
Bioamines	Bioamines	
Vesicle_0	Vesicle	

Product

Table 47: Properties of each product.

Id	Name	SBO
V_ntox_ba	V-ntox-ba	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{J2Sub}\left(\mathrm{k16}, [\mathrm{Bioamines}], \mathrm{g1643}, [\mathrm{Vesicle\_0}], \mathrm{g1644}\right) \tag{73}$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{74}$$

8.15 Reaction J17

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J17

Notes `Neurotoxin vesicle packaging`

Reaction equation

$$\text{Neurotoxins} + \text{Vesicle\_0} \xrightarrow{\text{Neurotoxins, Vesicle\_0, Neurotoxins, Vesicle\_0, Neurotoxins, Vesicle\_0, Neurotoxins, Vesi}} \quad (75)$$

Reactants

Table 48: Properties of each reactant.

Id	Name	SBO
Neurotoxins	Neurotoxins	
Vesicle_0	Vesicle	

Modifiers

Table 49: Properties of each modifier.

Id	Name	SBO
Neurotoxins	Neurotoxins	
Vesicle_0	Vesicle	
Neurotoxins	Neurotoxins	
Vesicle_0	Vesicle	
Neurotoxins	Neurotoxins	
Vesicle_0	Vesicle	
Neurotoxins	Neurotoxins	
Vesicle_0	Vesicle	
Neurotoxins	Neurotoxins	
Vesicle_0	Vesicle	
Neurotoxins	Neurotoxins	
Vesicle_0	Vesicle	
Neurotoxins	Neurotoxins	
Vesicle_0	Vesicle	
Neurotoxins	Neurotoxins	
Vesicle_0	Vesicle	
Neurotoxins	Neurotoxins	
Vesicle_0	Vesicle	

Product

Table 50: Properties of each product.

Id	Name	SBO
V_ntox_ba	V-ntox-ba	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{J2Sub}\left(\text{k17}, [\text{Neurotoxins}], \text{g1742}, [\text{Vesicle\_0}], \text{g1744}\right) \tag{76}$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \tag{77}$$

8.16 Reaction J18

This is an irreversible reaction of two reactants forming two products influenced by 18 modifiers.

Name J18

Notes DA quinone and superoxide radical synthesis

Reaction equation

$$\text{Dopamine} + \text{O2\_0} \xrightarrow{\text{Dopamine, O2\_0, Dopamine, O2\_0, Dopamine, O2\_0, Dopamine, O2\_0, Dopamine, O2\_0, Dopa}} \tag{78}$$

Reactants

Table 51: Properties of each reactant.

Id	Name	SBO
Dopamine	Dopamine	
O2_0	O2	

Modifiers

Table 52: Properties of each modifier.

Id	Name	SBO
Dopamine	Dopamine	

Id	Name	SBO
O2_0	O2	
Dopamine	Dopamine	
O2_0	O2	
Dopamine	Dopamine	
O2_0	O2	
Dopamine	Dopamine	
O2_0	O2	
Dopamine	Dopamine	
O2_0	O2	
Dopamine	Dopamine	
O2_0	O2	
Dopamine	Dopamine	
O2_0	O2	
Dopamine	Dopamine	
O2_0	O2	
Dopamine	Dopamine	
O2_0	O2	

Products

Table 53: Properties of each product.

Id	Name	SBO
DA_quinone	DA_quinone	
O2	O2-	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k18}, [\mathrm{Dopamine}], \mathrm{g186}, [\mathrm{O2\_0}], \mathrm{g1851}\right) \tag{79}$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{80}$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{81}$$

8.17 Reaction J19

This is an irreversible reaction of three reactants forming three products influenced by 37 modifiers.

Name J19

Notes DOPAL and H2O2 synthesis

Reaction equation

$$\text{Dopamine} + \text{O2\_0} + \text{H2O} \xrightarrow{\text{MAO, Dopamine, O2\_0, H2O, MAO, Dopamine, O2\_0, H2O, MAO, Dopamine, O2\_0, H}} \tag{82}$$

Reactants

Table 54: Properties of each reactant.

Id	Name	SBO
Dopamine	Dopamine	
O2_0	O2	
H2O	H2O	

Modifiers

Table 55: Properties of each modifier.

Id	Name	SBO
MAO	MAO	
Dopamine	Dopamine	
O2_0	O2	
H2O	H2O	
MAO	MAO	
Dopamine	Dopamine	
O2_0	O2	
H2O	H2O	
MAO	MAO	
Dopamine	Dopamine	
O2_0	O2	
H2O	H2O	
MAO	MAO	
Dopamine	Dopamine	
O2_0	O2	
H2O	H2O	
MAO	MAO	
Dopamine	Dopamine	
O2_0	O2	
H2O	H2O	
MAO	MAO	
Dopamine	Dopamine	
O2_0	O2	

Id	Name	SBO
H2O	H2O	
MAO	MAO	
Dopamine	Dopamine	
O2_0	O2	
H2O	H2O	
MAO	MAO	
Dopamine	Dopamine	
O2_0	O2	
H2O	H2O	
MAO	MAO	
Dopamine	Dopamine	
O2_0	O2	
H2O	H2O	
MAO	MAO	

Products

Table 56: Properties of each product.

Id	Name	SBO
NH3	NH3	
DOPAL	DOPAL	
H2O2	H2O2	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{Neuronal\_cytosol}) \cdot \mathrm{J3Sub1Mod}\,(\mathrm{k19}, [\mathrm{Dopamine}], \mathrm{g196}, [\mathrm{O2\_0}], \mathrm{g1951}, [\mathrm{H2O}], \mathrm{g1960}, [\mathrm{MAO}], \mathrm{g1953}) \tag{83}$$

$$\mathrm{J3Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}, \mathrm{X4}, \mathrm{G4}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \cdot \mathrm{X4}^{\mathrm{G4}} \tag{84}$$

$$\mathrm{J3Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}, \mathrm{X4}, \mathrm{G4}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \cdot \mathrm{X4}^{\mathrm{G4}} \tag{85}$$

8.18 Reaction J20

This is an irreversible reaction of two reactants forming three products influenced by 18 modifiers.

Name J20

Notes `Iron oxidation and formation of OH radicals`

Reaction equation

$$\mathrm{H2O2} + \mathrm{Fe2} \xrightarrow{\mathrm{H2O2,\ Fe2,\ H2O2,\ Fe2,\ H2O2,\ Fe2,\ H2O2,\ Fe2,\ H2O2,\ Fe2,\ H2O2,\ Fe2,\ H2O2,\ Fe2,\ H2O2,\ Fe2,\ H2}} \tag{86}$$

Reactants

Table 57: Properties of each reactant.

Id	Name	SBO
H2O2	H2O2	
Fe2	Fe2+	

Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
H2O2	H2O2	
Fe2	Fe2+	
H2O2	H2O2	
Fe2	Fe2+	
H2O2	H2O2	
Fe2	Fe2+	
H2O2	H2O2	
Fe2	Fe2+	
H2O2	H2O2	
Fe2	Fe2+	
H2O2	H2O2	
Fe2	Fe2+	
H2O2	H2O2	
Fe2	Fe2+	
H2O2	H2O2	
Fe2	Fe2+	
H2O2	H2O2	
Fe2	Fe2+	

Products

Table 59: Properties of each product.

Id	Name	SBO
Fe3	Fe3+	
OH_radical	OH_radical	
OH	OH-	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J2Sub}\,(\text{k20}, [\text{H2O2}], \text{g209}, [\text{Fe2}], \text{g2065}) \tag{87}$$

$$\text{J2Sub}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \tag{88}$$

$$\text{J2Sub}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \tag{89}$$

8.19 Reaction J21

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

Name J21

Notes Iron reduction

Reaction equation

$$\text{Fe3} \xrightarrow{\text{Fe3, Fe3, Fe3, Fe3, Fe3, Fe3, Fe3, Fe3, Fe3}} \text{Fe2} \tag{90}$$

Reactant

Table 60: Properties of each reactant.

Id	Name	SBO
Fe3	Fe3+	

Modifiers

Table 61: Properties of each modifier.

Id	Name	SBO
Fe3	Fe3+	

Id	Name	SBO
Fe3	Fe3+	
Fe3	Fe3+	
Fe3	Fe3+	
Fe3	Fe3+	
Fe3	Fe3+	
Fe3	Fe3+	
Fe3	Fe3+	
Fe3	Fe3+	

Product

Table 62: Properties of each product.

Id	Name	SBO
Fe2	Fe2+	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J1Sub}\left(\mathrm{k21}, [\mathrm{Fe3}], \mathrm{g2166}\right) \tag{91}$$

$$\mathrm{J1Sub}\left(\mathrm{K}, \mathrm{X}, \mathrm{G}\right) = \mathrm{K} \cdot \mathrm{X}^{\mathrm{G}} \tag{92}$$

$$\mathrm{J1Sub}\left(\mathrm{K}, \mathrm{X}, \mathrm{G}\right) = \mathrm{K} \cdot \mathrm{X}^{\mathrm{G}} \tag{93}$$

8.20 Reaction J22

This is an irreversible reaction of one reactant forming two products influenced by 19 modifiers.

Name J22

Notes `H2O2 depletion by catalase`

Reaction equation

$$\mathrm{H2O2} \xrightarrow{\text{Catalase, H2O2, Catalase, H2O2, Catalase, H2O2, Catalase, H2O2, Catalase, H2O2, Catalase, H2O2, Catala}} \tag{94}$$

Reactant

Table 63: Properties of each reactant.

Id	Name	SBO
H2O2	H2O2	

Modifiers

Table 64: Properties of each modifier.

Id	Name	SBO
Catalase	Catalase	
H2O2	H2O2	
Catalase	Catalase	
H2O2	H2O2	
Catalase	Catalase	
H2O2	H2O2	
Catalase	Catalase	
H2O2	H2O2	
Catalase	Catalase	
H2O2	H2O2	
Catalase	Catalase	
H2O2	H2O2	
Catalase	Catalase	
H2O2	H2O2	
Catalase	Catalase	
H2O2	H2O2	
Catalase	Catalase	
H2O2	H2O2	
Catalase	Catalase	

Products

Table 65: Properties of each product.

Id	Name	SBO
H2O	H2O	
O2_0	O2	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J1Sub1Mod}\,(\text{k22}, [\text{H2O2}], \text{g229}, [\text{Catalase}], \text{g2259}) \quad (95)$$

$$\text{J1Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (96)$$

$$\text{J1Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (97)$$

8.21 Reaction J23

This is an irreversible reaction of two reactants forming two products influenced by 28 modifiers.

Name J23

Notes `H2O2 depletion by GSH`

Reaction equation

$$\text{H2O2} + \text{GSH} \xrightarrow{\text{Gluta\_per, H2O2, GSH, Gluta\_per, H2O2, GSH, Gluta\_per, H2O2, GSH, Gluta\_per, H2O2, GSH, Gl}} \quad (98)$$

Reactants

Table 66: Properties of each reactant.

Id	Name	SBO
H2O2	H2O2	
GSH	GSH	

Modifiers

Table 67: Properties of each modifier.

Id	Name	SBO
Gluta_per	Gluta_per	
H2O2	H2O2	
GSH	GSH	
Gluta_per	Gluta_per	
H2O2	H2O2	
GSH	GSH	
Gluta_per	Gluta_per	
H2O2	H2O2	
GSH	GSH	
Gluta_per	Gluta_per	

Id	Name	SBO
H2O2	H2O2	
GSH	GSH	
Gluta_per	Gluta_per	
H2O2	H2O2	
GSH	GSH	
Gluta_per	Gluta_per	
H2O2	H2O2	
GSH	GSH	
Gluta_per	Gluta_per	
H2O2	H2O2	
GSH	GSH	
Gluta_per	Gluta_per	
H2O2	H2O2	
GSH	GSH	
Gluta_per	Gluta_per	
H2O2	H2O2	
GSH	GSH	
Gluta_per	Gluta_per	

Products

Table 68: Properties of each product.

Id	Name	SBO
H2O	H2O	
GSSG	GSSG	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub1Mod}\left(\mathrm{k23}, [\mathrm{H2O2}], \mathrm{g239}, [\mathrm{GSH}], \mathrm{g2362}, [\mathrm{Gluta\_per}], \mathrm{g2361}\right) \tag{99}$$

$$\mathrm{J2Sub1Mod}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \tag{100}$$

$$\mathrm{J2Sub1Mod}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \tag{101}$$

8.22 Reaction J24

This is an irreversible reaction of one reactant forming one product influenced by 19 modifiers.

Name J24

Reaction equation

$$\text{GSSG} \xrightarrow{\text{Gluta\_red, GSSG, Gluta\_red, GSSG, Gluta\_red, GSSG, Gluta\_red, GSSG, Gluta\_red, GSSG, Gluta\_red, GSS}} \tag{102}$$

Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
GSSG	GSSG	

Modifiers

Table 70: Properties of each modifier.

Id	Name	SBO
Gluta_red	Gluta_red	
GSSG	GSSG	
Gluta_red	Gluta_red	
GSSG	GSSG	
Gluta_red	Gluta_red	
GSSG	GSSG	
Gluta_red	Gluta_red	
GSSG	GSSG	
Gluta_red	Gluta_red	
GSSG	GSSG	
Gluta_red	Gluta_red	
GSSG	GSSG	
Gluta_red	Gluta_red	
GSSG	GSSG	
Gluta_red	Gluta_red	
GSSG	GSSG	
Gluta_red	Gluta_red	
GSSG	GSSG	
Gluta_red	Gluta_red	

Product

Table 71: Properties of each product.

Id	Name	SBO
GSH	GSH	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J1Sub1Mod}\,(\text{k24}, [\text{GSSG}], \text{g2463}, [\text{Gluta\_red}], \text{g2464}) \quad (103)$$

$$\text{J1Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (104)$$

$$\text{J1Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (105)$$

8.23 Reaction J25

This is an irreversible reaction of two reactants forming two products influenced by 28 modifiers.

Name J25

Notes DOPAC formation

Reaction equation

$$\text{DOPAL} + \text{NAD} \xrightarrow{\text{ALDH, DOPAL, NAD, ALDH, DOPAL, NAD, ALDH, DOPAL, NAD, ALDH, DOPAL, NAD, A}} \quad (106)$$

Reactants

Table 72: Properties of each reactant.

Id	Name	SBO
DOPAL	DOPAL	
NAD	NAD+	

Modifiers

Table 73: Properties of each modifier.

Id	Name	SBO
ALDH	ALDH	
DOPAL	DOPAL	
NAD	NAD+	
ALDH	ALDH	
DOPAL	DOPAL	
NAD	NAD+	
ALDH	ALDH	
DOPAL	DOPAL	
NAD	NAD+	
ALDH	ALDH	
DOPAL	DOPAL	
NAD	NAD+	
ALDH	ALDH	
DOPAL	DOPAL	
NAD	NAD+	
ALDH	ALDH	
DOPAL	DOPAL	
NAD	NAD+	
ALDH	ALDH	
DOPAL	DOPAL	
NAD	NAD+	
ALDH	ALDH	
DOPAL	DOPAL	
NAD	NAD+	
ALDH	ALDH	
DOPAL	DOPAL	
NAD	NAD+	
ALDH	ALDH	

Products

Table 74: Properties of each product.

Id	Name	SBO
DOPAC	DOPAC	
NADH	NADH	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J2Sub1Mod}\,(\text{k25}, [\text{DOPAL}], \text{g2552}, [\text{NAD}], \text{g2556}, [\text{ALDH}], \text{g2555}) \tag{107}$$

$$\text{J2Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}, \text{X3}, \text{G3}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \cdot \text{X3}^{\text{G3}} \tag{108}$$

$$\text{J2Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}, \text{X3}, \text{G3}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \cdot \text{X3}^{\text{G3}} \tag{109}$$

8.24 Reaction J26f

This is an irreversible reaction of two reactants forming two products influenced by 28 modifiers.

Name J26f

Notes `Forward ubiquitination tag 2`

Reaction equation

$$\text{Ub\_E1} + \text{UbcH8\_Ub} \xrightarrow{\text{ATP, Ub\_E1, UbcH8\_Ub, ATP, Ub\_E1, UbcH8\_Ub, ATP, Ub\_E1, UbcH8\_Ub, ATP, Ub\_E1, U}} \tag{110}$$

Reactants

Table 75: Properties of each reactant.

Id	Name	SBO
Ub_E1	Ub-E1	
UbcH8_Ub	UbcH8-Ub	

Modifiers

Table 76: Properties of each modifier.

Id	Name	SBO
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8_Ub	UbcH8-Ub	
ATP	ATP	

Id	Name	SBO
Ub_E1	Ub-E1	
UbcH8_Ub	UbcH8-Ub	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8_Ub	UbcH8-Ub	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8_Ub	UbcH8-Ub	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8_Ub	UbcH8-Ub	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8_Ub	UbcH8-Ub	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8_Ub	UbcH8-Ub	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8_Ub	UbcH8-Ub	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8_Ub	UbcH8-Ub	
ATP	ATP	

Products

Table 77: Properties of each product.

Id	Name	SBO
E1	E1	
UbcH8ub2	UbcH8ub2	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub1Mod}\left(\mathrm{k26f}, [\mathrm{Ub\_E1}], \mathrm{g26f16}, [\mathrm{UbcH8\_Ub}], \mathrm{g26f18}, [\mathrm{ATP}], \mathrm{g26f15}\right) \tag{111}$$

$$\mathrm{J2Sub1Mod}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \tag{112}$$

$$\mathrm{J2Sub1Mod}(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \quad (113)$$

8.25 Reaction J26r

This is an irreversible reaction of one reactant forming two products influenced by 19 modifiers.

Name J26r

Notes `Reverse ubiquitination tag 2`

Reaction equation

$$\mathrm{UbcH8ub2} \xrightarrow{\mathrm{UCH\_L1},\ \mathrm{UbcH8ub2},\ \mathrm{UCH\_L1},\ \mathrm{UbcH8ub2},\ \mathrm{UCH\_L1},\ \mathrm{UbcH8ub2},\ \mathrm{UCH\_L1},\ \mathrm{UbcH8ub2},\ \mathrm{UCH\_L1},\ \mathrm{Ubc}} \quad (114)$$

Reactant

Table 78: Properties of each reactant.

Id	Name	SBO
UbcH8ub2	UbcH8ub2	

Modifiers

Table 79: Properties of each modifier.

Id	Name	SBO
UCH_L1	UCH-L1	
UbcH8ub2	UbcH8ub2	
UCH_L1	UCH-L1	
UbcH8ub2	UbcH8ub2	
UCH_L1	UCH-L1	
UbcH8ub2	UbcH8ub2	
UCH_L1	UCH-L1	
UbcH8ub2	UbcH8ub2	
UCH_L1	UCH-L1	
UbcH8ub2	UbcH8ub2	
UCH_L1	UCH-L1	
UbcH8ub2	UbcH8ub2	
UCH_L1	UCH-L1	
UbcH8ub2	UbcH8ub2	
UCH_L1	UCH-L1	
UbcH8ub2	UbcH8ub2	

Id	Name	SBO
UCH_L1	UCH-L1	
UbcH8ub2	UbcH8ub2	
UCH_L1	UCH-L1	

Products

Table 80: Properties of each product.

Id	Name	SBO
UbcH8	UbcH8	
Ubiquitin	Ubiquitin	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J1Sub1Mod}\,(\text{k26r}, [\text{UbcH8ub2}], \text{g26r68}, [\text{UCH\_L1}], \text{g26r30}) \tag{115}$$

$$\text{J1Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \tag{116}$$

$$\text{J1Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \tag{117}$$

8.26 Reaction J27f

This is an irreversible reaction of two reactants forming two products influenced by 28 modifiers.

Name J27f

Notes Forward ubiquitination tag 3

Reaction equation

$$\text{Ub\_E1} + \text{UbcH8ub2} \xrightarrow{\text{ATP, Ub\_E1, UbcH8ub2, ATP, Ub\_E1, UbcH8ub2, ATP, Ub\_E1, UbcH8ub2, ATP, Ub\_E1, Ub}} \tag{118}$$

Reactants

Table 81: Properties of each reactant.

Id	Name	SBO
Ub_E1	Ub-E1	
UbcH8ub2	UbcH8ub2	

Modifiers

Table 82: Properties of each modifier.

Id	Name	SBO
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub2	UbcH8ub2	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub2	UbcH8ub2	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub2	UbcH8ub2	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub2	UbcH8ub2	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub2	UbcH8ub2	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub2	UbcH8ub2	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub2	UbcH8ub2	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub2	UbcH8ub2	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub2	UbcH8ub2	
ATP	ATP	

Products

Table 83: Properties of each product.

Id	Name	SBO
E1	E1	
UbcH8ub3	UbcH8ub3	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J2Sub1Mod}\,(\text{k27f}, [\text{Ub\_E1}], \text{g27f16}, [\text{UbcH8ub2}], \text{g27f68}, [\text{ATP}], \text{g27f15}) \tag{119}$$

$$\text{J2Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}, \text{X3}, \text{G3}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \cdot \text{X3}^{\text{G3}} \tag{120}$$

$$\text{J2Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}, \text{X3}, \text{G3}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \cdot \text{X3}^{\text{G3}} \tag{121}$$

8.27 Reaction J27r

This is an irreversible reaction of one reactant forming two products influenced by 19 modifiers.

Name J27r

Notes Reverse ubiquitination tag 3

Reaction equation

$$\text{UbcH8ub3} \xrightarrow{\text{UCH\_L1, UbcH8ub3, UCH\_L1, UbcH8ub3, UCH\_L1, UbcH8ub3, UCH\_L1, UbcH8ub3, UCH\_L1, Ubc}} \tag{122}$$

Reactant

Table 84: Properties of each reactant.

Id	Name	SBO
UbcH8ub3	UbcH8ub3	

Modifiers

Table 85: Properties of each modifier.

Id	Name	SBO
UCH_L1	UCH-L1	
UbcH8ub3	UbcH8ub3	
UCH_L1	UCH-L1	
UbcH8ub3	UbcH8ub3	
UCH_L1	UCH-L1	
UbcH8ub3	UbcH8ub3	
UCH_L1	UCH-L1	
UbcH8ub3	UbcH8ub3	
UCH_L1	UCH-L1	
UbcH8ub3	UbcH8ub3	
UCH_L1	UCH-L1	
UbcH8ub3	UbcH8ub3	
UCH_L1	UCH-L1	
UbcH8ub3	UbcH8ub3	
UCH_L1	UCH-L1	
UbcH8ub3	UbcH8ub3	
UCH_L1	UCH-L1	
UbcH8ub3	UbcH8ub3	
UCH_L1	UCH-L1	

Products

Table 86: Properties of each product.

Id	Name	SBO
UbcH8	UbcH8	
Ubiquitin	Ubiquitin	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J1Sub1Mod}\left(\mathrm{k27r}, [\mathrm{UbcH8ub3}], \mathrm{g27r69}, [\mathrm{UCH\_L1}], \mathrm{g27r30}\right) \tag{123}$$

$$\mathrm{J1Sub1Mod}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{124}$$

$$\mathrm{J1Sub1Mod}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{125}$$

8.28 Reaction J28f

This is an irreversible reaction of two reactants forming two products influenced by 28 modifiers.

Name J28f

Notes Forward ubiquitination tag 4

Reaction equation

$$\text{Ub\_E1} + \text{UbcH8ub3} \xrightarrow{\text{ATP, Ub\_E1, UbcH8ub3, ATP, Ub\_E1, UbcH8ub3, ATP, Ub\_E1, UbcH8ub3, ATP, Ub\_E1, Ub}} \tag{126}$$

Reactants

Table 87: Properties of each reactant.

Id	Name	SBO
Ub_E1	Ub-E1	
UbcH8ub3	UbcH8ub3	

Modifiers

Table 88: Properties of each modifier.

Id	Name	SBO
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub3	UbcH8ub3	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub3	UbcH8ub3	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub3	UbcH8ub3	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub3	UbcH8ub3	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub3	UbcH8ub3	
ATP	ATP	
Ub_E1	Ub-E1	

Id	Name	SBO
UbcH8ub3	UbcH8ub3	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub3	UbcH8ub3	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub3	UbcH8ub3	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH8ub3	UbcH8ub3	
ATP	ATP	

Products

Table 89: Properties of each product.

Id	Name	SBO
E1	E1	
UbcH8ub4	UbcH8ub4	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \mathrm{vol}\,(\mathrm{Neuronal\_cytosol}) \cdot \mathrm{J2Sub1Mod}\,(\mathrm{k28f}, [\mathrm{Ub\_E1}], \mathrm{g28f16}, [\mathrm{UbcH8ub3}], \mathrm{g28f69}, [\mathrm{ATP}], \mathrm{g28f15}) \tag{127}$$

$$\mathrm{J2Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \tag{128}$$

$$\mathrm{J2Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \tag{129}$$

8.29 Reaction J28r

This is an irreversible reaction of one reactant forming two products influenced by 19 modifiers.

Name J28r

Notes Reverse ubiquitination tag 4

Reaction equation

$$\text{UbcH8ub4} \xrightarrow{\text{UCH\_L1, UbcH8ub4, UCH\_L1, UbcH8ub4, UCH\_L1, UbcH8ub4, UCH\_L1, UbcH8ub4, UCH\_L1, Ubc}} \quad (130)$$

Reactant

Table 90: Properties of each reactant.

Id	Name	SBO
UbcH8ub4	UbcH8ub4	

Modifiers

Table 91: Properties of each modifier.

Id	Name	SBO
UCH_L1	UCH-L1	
UbcH8ub4	UbcH8ub4	
UCH_L1	UCH-L1	
UbcH8ub4	UbcH8ub4	
UCH_L1	UCH-L1	
UbcH8ub4	UbcH8ub4	
UCH_L1	UCH-L1	
UbcH8ub4	UbcH8ub4	
UCH_L1	UCH-L1	
UbcH8ub4	UbcH8ub4	
UCH_L1	UCH-L1	
UbcH8ub4	UbcH8ub4	
UCH_L1	UCH-L1	
UbcH8ub4	UbcH8ub4	
UCH_L1	UCH-L1	
UbcH8ub4	UbcH8ub4	
UCH_L1	UCH-L1	
UbcH8ub4	UbcH8ub4	
UCH_L1	UCH-L1	

Products

Table 92: Properties of each product.

Id	Name	SBO
UbcH8	UbcH8	
Ubiquitin	Ubiquitin	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \mathrm{vol}\,(\mathrm{Neuronal\_cytosol}) \cdot \mathrm{J1Sub1Mod}\,(\mathrm{k28r}, [\mathrm{UbcH8ub4}], \mathrm{g28r70}, [\mathrm{UCH\_L1}], \mathrm{g28r30}) \tag{131}$$

$$\mathrm{J1Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{132}$$

$$\mathrm{J1Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{133}$$

8.30 Reaction J29

This is an irreversible reaction of two reactants forming two products influenced by 28 modifiers.

Name J29

Notes UbcH13/Uev1a conjugation

Reaction equation

$$\mathrm{Ub\_E1} + \mathrm{UbcH13\_Uev1a} \xrightarrow{\mathrm{ATP,\ Ub\_E1,\ UbcH13\_Uev1a,\ ATP,\ Ub\_E1,\ UbcH13\_Uev1a,\ ATP,\ Ub\_E1,\ UbcH13\_Uev1}} \tag{134}$$

Reactants

Table 93: Properties of each reactant.

Id	Name	SBO
Ub_E1	Ub-E1	
UbcH13_Uev1a	UbcH13/Uev1a	

Modifiers

Table 94: Properties of each modifier.

Id	Name	SBO
ATP	ATP	
Ub_E1	Ub-E1	
UbcH13_Uev1a	UbcH13/Uev1a	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH13_Uev1a	UbcH13/Uev1a	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH13_Uev1a	UbcH13/Uev1a	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH13_Uev1a	UbcH13/Uev1a	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH13_Uev1a	UbcH13/Uev1a	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH13_Uev1a	UbcH13/Uev1a	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH13_Uev1a	UbcH13/Uev1a	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH13_Uev1a	UbcH13/Uev1a	
ATP	ATP	
Ub_E1	Ub-E1	
UbcH13_Uev1a	UbcH13/Uev1a	
ATP	ATP	

Products

Table 95: Properties of each product.

Id	Name	SBO
E1	E1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J2Sub1Mod}\,(\text{k29}, [\text{Ub\_E1}], \text{g2916}, [\text{UbcH13\_Uev1a}], \text{g2971}, [\text{ATP}], \text{g2915}) \tag{135}$$

$$\text{J2Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}, \text{X3}, \text{G3}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \cdot \text{X3}^{\text{G3}} \tag{136}$$

$$\text{J2Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}, \text{X3}, \text{G3}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \cdot \text{X3}^{\text{G3}} \tag{137}$$

8.31 Reaction J30

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J30

Notes `Asyn ligation to UCH-L1`

Reaction equation

$$\text{Alpha\_synuclein} + \text{UCH\_L1} \xrightarrow{\text{Alpha\_synuclein, UCH\_L1, Alpha\_synuclein, UCH\_L1, Alpha\_synuclein, UCH\_L1, Al}} \tag{138}$$

Reactants

Table 96: Properties of each reactant.

Id	Name	SBO
`Alpha_synuclein`	Alpha_synuclein	
`UCH_L1`	UCH-L1	

Modifiers

Table 97: Properties of each modifier.

Id	Name	SBO
`Alpha_synuclein`	Alpha_synuclein	
`UCH_L1`	UCH-L1	
`Alpha_synuclein`	Alpha_synuclein	
`UCH_L1`	UCH-L1	

Id	Name	SBO
Alpha_synuclein	Alpha_synuclein	
UCH_L1	UCH-L1	
Alpha_synuclein	Alpha_synuclein	
UCH_L1	UCH-L1	
Alpha_synuclein	Alpha_synuclein	
UCH_L1	UCH-L1	
Alpha_synuclein	Alpha_synuclein	
UCH_L1	UCH-L1	
Alpha_synuclein	Alpha_synuclein	
UCH_L1	UCH-L1	
Alpha_synuclein	Alpha_synuclein	
UCH_L1	UCH-L1	
Alpha_synuclein	Alpha_synuclein	
UCH_L1	UCH-L1	

Product

Table 98: Properties of each product.

Id	Name	SBO
asyn_UCH_L1	asyn-UCH-L1	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \mathrm{vol}\,(\mathrm{Neuronal\_cytosol}) \cdot \mathrm{J2Sub}\,(\mathrm{k30}, [\mathrm{Alpha\_synuclein}], \mathrm{g301}, [\mathrm{UCH\_L1}], \mathrm{g3030}) \quad (139)$$

$$\mathrm{J2Sub}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (140)$$

$$\mathrm{J2Sub}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (141)$$

8.32 Reaction J31

This is an irreversible reaction of two reactants forming three products influenced by 18 modifiers.

Name J31

Notes Alpha synuclein K63 ubiquitination

Reaction equation

$$UbcH13\_Uev1a\_ub + asyn\_UCH\_L1 \xrightarrow{UbcH13\_Uev1a\_ub,\ asyn\_UCH\_L1,\ UbcH13\_Uev1a\_ub,\ asyn\_UCH\_L1,\ UbcH1} \quad (142)$$

Reactants

Table 99: Properties of each reactant.

Id	Name	SBO
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
asyn_UCH_L1	asyn-UCH-L1	

Modifiers

Table 100: Properties of each modifier.

Id	Name	SBO
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
asyn_UCH_L1	asyn-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
asyn_UCH_L1	asyn-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
asyn_UCH_L1	asyn-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
asyn_UCH_L1	asyn-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
asyn_UCH_L1	asyn-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
asyn_UCH_L1	asyn-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
asyn_UCH_L1	asyn-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
asyn_UCH_L1	asyn-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
asyn_UCH_L1	asyn-UCH-L1	

Products

Table 101: Properties of each product.

Id	Name	SBO
UbcH13_Uev1a	UbcH13/Uev1a	
UCH_L1	UCH-L1	
asyn_ub	asyn-ub	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k31}, [\mathrm{UbcH13\_Uev1a\_ub}], \mathrm{g3172}, [\mathrm{asyn\_UCH\_L1}], \mathrm{g3173}\right) \tag{143}$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{144}$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{145}$$

8.33 Reaction J32

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J32

Notes Asyn reaction with asyn-ub to form protofibrils

Reaction equation

$$\mathrm{Alpha\_synuclein} + \mathrm{asyn\_ub} \xrightarrow{\mathrm{Alpha\_synuclein,\ asyn\_ub,\ Alpha\_synuclein,\ asyn\_ub,\ Alpha\_synuclein,\ asyn\_ub,\ Alpha\_}} \tag{146}$$

Reactants

Table 102: Properties of each reactant.

Id	Name	SBO
Alpha_synuclein	Alpha_synuclein	
asyn_ub	asyn-ub	

Modifiers

Table 103: Properties of each modifier.

Id	Name	SBO
Alpha_synuclein	Alpha_synuclein	
asyn_ub	asyn-ub	
Alpha_synuclein	Alpha_synuclein	
asyn_ub	asyn-ub	
Alpha_synuclein	Alpha_synuclein	
asyn_ub	asyn-ub	
Alpha_synuclein	Alpha_synuclein	
asyn_ub	asyn-ub	
Alpha_synuclein	Alpha_synuclein	
asyn_ub	asyn-ub	
Alpha_synuclein	Alpha_synuclein	
asyn_ub	asyn-ub	
Alpha_synuclein	Alpha_synuclein	
asyn_ub	asyn-ub	
Alpha_synuclein	Alpha_synuclein	
asyn_ub	asyn-ub	
Alpha_synuclein	Alpha_synuclein	
asyn_ub	asyn-ub	

Product

Table 104: Properties of each product.

Id	Name	SBO
Protofibril	Protofibril	

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k32}, [\mathrm{Alpha\_synuclein}], \mathrm{g321}, [\mathrm{asyn\_ub}], \mathrm{g3274}\right) \quad (147)$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (148)$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (149)$$

8.34 Reaction J33

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J33

Notes Protofibril ligation to UCH-L1

Reaction equation

$$\text{Protofibril} + \text{UCH\_L1} \xrightarrow{\text{Protofibril, UCH\_L1, Protofibril, UCH\_L1, Protofibril, UCH\_L1, Protofibril, UCH\_L1, Protof}} \quad (150)$$

Reactants

Table 105: Properties of each reactant.

Id	Name	SBO
Protofibril	Protofibril	
UCH_L1	UCH-L1	

Modifiers

Table 106: Properties of each modifier.

Id	Name	SBO
Protofibril	Protofibril	
UCH_L1	UCH-L1	
Protofibril	Protofibril	
UCH_L1	UCH-L1	
Protofibril	Protofibril	
UCH_L1	UCH-L1	
Protofibril	Protofibril	
UCH_L1	UCH-L1	
Protofibril	Protofibril	
UCH_L1	UCH-L1	
Protofibril	Protofibril	
UCH_L1	UCH-L1	
Protofibril	Protofibril	
UCH_L1	UCH-L1	
Protofibril	Protofibril	
UCH_L1	UCH-L1	
Protofibril	Protofibril	

Id	Name	SBO
UCH_L1	UCH-L1	

Product

Table 107: Properties of each product.

Id	Name	SBO
Protofibril_UCH_L1	Protofibril-UCH-L1	

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \text{vol}\left(\text{Neuronal\_cytosol}\right) \cdot \text{J2Sub}\left(\text{k33}, [\text{Protofibril}], \text{g332}, [\text{UCH\_L1}], \text{g3330}\right) \quad (151)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (152)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (153)$$

8.35 Reaction J34

This is an irreversible reaction of two reactants forming three products influenced by 18 modifiers.

Name J34

Notes Protofibril K63 ubiquitination

Reaction equation

$$\text{UbcH13\_Uev1a\_ub} + \text{Protofibril\_UCH\_L1} \xrightarrow{\text{UbcH13\_Uev1a\_ub, Protofibril\_UCH\_L1, UbcH13\_Uev1a\_ub, Protofibril\_}} \quad (154)$$

Reactants

Table 108: Properties of each reactant.

Id	Name	SBO
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Protofibril_UCH_L1	Protofibril-UCH-L1	

Modifiers

Table 109: Properties of each modifier.

Id	Name	SBO
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Protofibril_UCH_L1	Protofibril-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Protofibril_UCH_L1	Protofibril-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Protofibril_UCH_L1	Protofibril-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Protofibril_UCH_L1	Protofibril-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Protofibril_UCH_L1	Protofibril-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Protofibril_UCH_L1	Protofibril-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Protofibril_UCH_L1	Protofibril-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Protofibril_UCH_L1	Protofibril-UCH-L1	
UbcH13_Uev1a_ub	UbcH13/Uev1a-ub	
Protofibril_UCH_L1	Protofibril-UCH-L1	

Products

Table 110: Properties of each product.

Id	Name	SBO
UbcH13_Uev1a	UbcH13/Uev1a	
UCH_L1	UCH-L1	
Protofibril_Ub	Protofibril-Ub	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k34}, [\mathrm{UbcH13\_Uev1a\_ub}], \mathrm{g3472}, [\mathrm{Protofibril\_UCH\_L1}], \mathrm{g3475}\right) \tag{155}$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{156}$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{157}$$

8.36 Reaction J35

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J35

Notes `Protofibril reaction with protofibril-ub to form fibrils`

Reaction equation

$$\text{Protofibril} + \text{Protofibril\_Ub} \xrightarrow{\text{Protofibril, Protofibril\_Ub, Protofibril, Protofibril\_Ub, Protofibril, Protofibril\_Ub, Protofi}} \tag{158}$$

Reactants

Table 111: Properties of each reactant.

Id	Name	SBO
Protofibril	Protofibril	
Protofibril_Ub	Protofibril-Ub	

Modifiers

Table 112: Properties of each modifier.

Id	Name	SBO
Protofibril	Protofibril	
Protofibril_Ub	Protofibril-Ub	
Protofibril	Protofibril	
Protofibril_Ub	Protofibril-Ub	
Protofibril	Protofibril	
Protofibril_Ub	Protofibril-Ub	
Protofibril	Protofibril	
Protofibril_Ub	Protofibril-Ub	
Protofibril	Protofibril	
Protofibril_Ub	Protofibril-Ub	
Protofibril	Protofibril	
Protofibril_Ub	Protofibril-Ub	
Protofibril	Protofibril	
Protofibril_Ub	Protofibril-Ub	
Protofibril	Protofibril	
Protofibril_Ub	Protofibril-Ub	
Protofibril	Protofibril	

Id	Name	SBO
Protofibril_Ub	Protofibril-Ub	

Product

Table 113: Properties of each product.

Id	Name	SBO
Fibril	Fibril	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \text{vol}\left(\text{Neuronal\_cytosol}\right) \cdot \text{J2Sub}\left(\text{k35}, [\text{Protofibril}], \text{g352}, [\text{Protofibril\_Ub}], \text{g3576}\right) \quad (159)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (160)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (161)$$

8.37 Reaction J36

This is an irreversible reaction of one reactant forming one product influenced by 19 modifiers.

Name J36

Notes Lysosomal degradation of autophagosome

Reaction equation

$$\text{Autophagosome\_0} \xrightarrow{\text{Lysosome\_0, Autophagosome\_0, Lysosome\_0, Autophagosome\_0, Lysosome\_0, Autophagosome}} \quad (162)$$

Reactant

Table 114: Properties of each reactant.

Id	Name	SBO
Autophagosome_0	Autophagosome	

Modifiers

Table 115: Properties of each modifier.

Id	Name	SBO
Lysosome_0	Lysosome	
Autophagosome_0	Autophagosome	
Lysosome_0	Lysosome	
Autophagosome_0	Autophagosome	
Lysosome_0	Lysosome	
Autophagosome_0	Autophagosome	
Lysosome_0	Lysosome	
Autophagosome_0	Autophagosome	
Lysosome_0	Lysosome	
Autophagosome_0	Autophagosome	
Lysosome_0	Lysosome	
Autophagosome_0	Autophagosome	
Lysosome_0	Lysosome	
Autophagosome_0	Autophagosome	
Lysosome_0	Lysosome	
Autophagosome_0	Autophagosome	
Lysosome_0	Lysosome	
Autophagosome_0	Autophagosome	
Lysosome_0	Lysosome	

Product

Table 116: Properties of each product.

Id	Name	SBO
Fragments	Fragments	

Kinetic Law

Derived unit contains undeclared units

$$v_{37} = \mathrm{J1Sub1Mod}\left(\mathrm{k36}, [\mathrm{Autophagosome\_0}], \mathrm{g3679}, [\mathrm{Lysosome\_0}], \mathrm{g3677}\right) \quad (163)$$

$$\mathrm{J1Sub1Mod}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (164)$$

8.38 Reaction J37

This is an irreversible reaction of two reactants forming two products influenced by 18 modifiers.

Name J37

Notes `Asyn K48 ubiquitination`

Reaction equation

$$\text{UbcH8ub4} + \text{asyn\_UCH\_L1} \xrightarrow{\text{UbcH8ub4, asyn\_UCH\_L1, UbcH8ub4, asyn\_UCH\_L1, UbcH8ub4, asyn\_UCH\_L1, Ub}} \tag{165}$$

Reactants

Table 117: Properties of each reactant.

Id	Name	SBO
UbcH8ub4	UbcH8ub4	
asyn_UCH_L1	asyn-UCH-L1	

Modifiers

Table 118: Properties of each modifier.

Id	Name	SBO
UbcH8ub4	UbcH8ub4	
asyn_UCH_L1	asyn-UCH-L1	
UbcH8ub4	UbcH8ub4	
asyn_UCH_L1	asyn-UCH-L1	
UbcH8ub4	UbcH8ub4	
asyn_UCH_L1	asyn-UCH-L1	
UbcH8ub4	UbcH8ub4	
asyn_UCH_L1	asyn-UCH-L1	
UbcH8ub4	UbcH8ub4	
asyn_UCH_L1	asyn-UCH-L1	
UbcH8ub4	UbcH8ub4	
asyn_UCH_L1	asyn-UCH-L1	
UbcH8ub4	UbcH8ub4	
asyn_UCH_L1	asyn-UCH-L1	
UbcH8ub4	UbcH8ub4	
asyn_UCH_L1	asyn-UCH-L1	
UbcH8ub4	UbcH8ub4	

Id	Name	SBO
asyn_UCH_L1	asyn-UCH-L1	

Products

Table 119: Properties of each product.

Id	Name	SBO
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	
UbcH8	UbcH8	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J2Sub}\,(\text{k37}, [\text{UbcH8ub4}], \text{g3770}, [\text{asyn\_UCH\_L1}], \text{g3773}) \quad (166)$$

$$\text{J2Sub}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (167)$$

$$\text{J2Sub}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (168)$$

8.39 Reaction J38

This is an irreversible reaction of one reactant forming three products influenced by 39 modifiers.

Name J38

Notes Proteasomal degradation of UCH-L1-asyn-ub4

Reaction equation

$$\text{UCH\_L1\_asyn\_ub4} \xrightarrow{\text{Proteasome\_0, ATP, UCH\_L1, UCH\_L1\_asyn\_ub4, Proteasome\_0, ATP, UCH\_L1, UCH\_L1\_asyn}} \quad (169)$$

Reactant

Table 120: Properties of each reactant.

Id	Name	SBO
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	

Modifiers

Table 121: Properties of each modifier.

Id	Name	SBO
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	
Proteasome_0	Proteasome	
ATP	ATP	
UCH_L1	UCH-L1	
UCH_L1_asyn_ub4	UCH-L1-asyn-ub4	
Proteasome_0	Proteasome	
ATP	ATP	

Id	Name	SBO
UCH_L1	UCH-L1	

Products

Table 122: Properties of each product.

Id	Name	SBO
Fragments	Fragments	
UCH_L1	UCH-L1	
Ubiquitin	Ubiquitin	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J1Sub3Mod}\,(\text{k38}, [\text{UCH\_L1\_asyn\_ub4}], \text{g3878}, [\text{Proteasome\_0}], \text{g3812}, [\text{ATP}], \text{g3815}, [\text{UCH\_L1}], \text{g3830}) \quad (170)$$

$$\text{J1Sub3Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}, \text{X3}, \text{G3}, \text{X4}, \text{G4}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \cdot \text{X3}^{\text{G3}} \cdot \text{X4}^{\text{G4}} \quad (171)$$

$$\text{J1Sub3Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}, \text{X3}, \text{G3}, \text{X4}, \text{G4}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \cdot \text{X3}^{\text{G3}} \cdot \text{X4}^{\text{G4}} \quad (172)$$

8.40 Reaction J43

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J43

Notes hsc70-asyn formation

Reaction equation

$$\text{Alpha\_synuclein} + \text{Hsc70} \xrightarrow{\text{Alpha\_synuclein, Hsc70, Alpha\_synuclein, Hsc70, Alpha\_synuclein, Hsc70, Alpha\_synuc}} \quad (173)$$

Reactants

Table 123: Properties of each reactant.

Id	Name	SBO
Alpha_synuclein	Alpha_synuclein	
Hsc70	Hsc70	

Modifiers

Table 124: Properties of each modifier.

Id	Name	SBO
Alpha_synuclein	Alpha_synuclein	
Hsc70	Hsc70	
Alpha_synuclein	Alpha_synuclein	
Hsc70	Hsc70	
Alpha_synuclein	Alpha_synuclein	
Hsc70	Hsc70	
Alpha_synuclein	Alpha_synuclein	
Hsc70	Hsc70	
Alpha_synuclein	Alpha_synuclein	
Hsc70	Hsc70	
Alpha_synuclein	Alpha_synuclein	
Hsc70	Hsc70	
Alpha_synuclein	Alpha_synuclein	
Hsc70	Hsc70	
Alpha_synuclein	Alpha_synuclein	
Hsc70	Hsc70	
Alpha_synuclein	Alpha_synuclein	
Hsc70	Hsc70	

Product

Table 125: Properties of each product.

Id	Name	SBO
Hsc70_asyn	Hsc70-asyn	

Kinetic Law

Derived unit contains undeclared units

$$v_{40} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k43}, [\mathrm{Alpha\_synuclein}], \mathrm{g431}, [\mathrm{Hsc70}], \mathrm{g4384}\right) \quad (174)$$

$$\mathrm{J2Sub}\left(\mathrm{K},\mathrm{X1},\mathrm{G1},\mathrm{X2},\mathrm{G2}\right) = \mathrm{K}\cdot\mathrm{X1}^{\mathrm{G1}}\cdot\mathrm{X2}^{\mathrm{G2}} \tag{175}$$

$$\mathrm{J2Sub}\left(\mathrm{K},\mathrm{X1},\mathrm{G1},\mathrm{X2},\mathrm{G2}\right) = \mathrm{K}\cdot\mathrm{X1}^{\mathrm{G1}}\cdot\mathrm{X2}^{\mathrm{G2}} \tag{176}$$

8.41 Reaction J44

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J44

Notes Hsc70-protofibril formation

Reaction equation

$$\mathrm{Protofibril} + \mathrm{Hsc70} \xrightarrow{\mathrm{Protofibril,\ Hsc70,\ Protofibril,\ Hsc70,\ Protofibril,\ Hsc70,\ Protofibril,\ Hsc70,\ Protofibril,\ Hsc70,}} \tag{177}$$

Reactants

Table 126: Properties of each reactant.

Id	Name	SBO
Protofibril	Protofibril	
Hsc70	Hsc70	

Modifiers

Table 127: Properties of each modifier.

Id	Name	SBO
Protofibril	Protofibril	
Hsc70	Hsc70	
Protofibril	Protofibril	
Hsc70	Hsc70	
Protofibril	Protofibril	
Hsc70	Hsc70	
Protofibril	Protofibril	
Hsc70	Hsc70	
Protofibril	Protofibril	
Hsc70	Hsc70	
Protofibril	Protofibril	
Hsc70	Hsc70	

Id	Name	SBO
Protofibril	Protofibril	
Hsc70	Hsc70	
Protofibril	Protofibril	
Hsc70	Hsc70	
Protofibril	Protofibril	
Hsc70	Hsc70	

Product

Table 128: Properties of each product.

Id	Name	SBO
Hsc70_Protofibril	Hsc70-Protofibril	

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = \text{vol}\left(\text{Neuronal\_cytosol}\right) \cdot \text{J2Sub}\left(\text{k44}, [\text{Protofibril}], \text{g442}, [\text{Hsc70}], \text{g4484}\right) \quad (178)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (179)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (180)$$

8.42 Reaction J45

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J45

Notes Hsc70-fibril formation

Reaction equation

$$\text{Fibril} + \text{Hsc70} \xrightarrow{\text{Fibril, Hsc70, Fibril, Hsc70, Fibril, Hsc70, Fibril, Hsc70, Fibril, Hsc70, Fibril, Hsc70, Fibril, Hsc70}} \quad (181)$$

Reactants

Table 129: Properties of each reactant.

Id	Name	SBO
Fibril	Fibril	
Hsc70	Hsc70	

Modifiers

Table 130: Properties of each modifier.

Id	Name	SBO
Fibril	Fibril	
Hsc70	Hsc70	
Fibril	Fibril	
Hsc70	Hsc70	
Fibril	Fibril	
Hsc70	Hsc70	
Fibril	Fibril	
Hsc70	Hsc70	
Fibril	Fibril	
Hsc70	Hsc70	
Fibril	Fibril	
Hsc70	Hsc70	
Fibril	Fibril	
Hsc70	Hsc70	
Fibril	Fibril	
Hsc70	Hsc70	
Fibril	Fibril	
Hsc70	Hsc70	

Product

Table 131: Properties of each product.

Id	Name	SBO
Hsc70_fibril	Hsc70-fibril	

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k45}, [\mathrm{Fibril}], \mathrm{g453}, [\mathrm{Hsc70}], \mathrm{g4584}\right) \tag{182}$$

$$\mathrm{J2Sub}(\mathrm{K},\mathrm{X1},\mathrm{G1},\mathrm{X2},\mathrm{G2}) = \mathrm{K}\cdot\mathrm{X1}^{\mathrm{G1}}\cdot\mathrm{X2}^{\mathrm{G2}} \tag{183}$$

$$\mathrm{J2Sub}(\mathrm{K},\mathrm{X1},\mathrm{G1},\mathrm{X2},\mathrm{G2}) = \mathrm{K}\cdot\mathrm{X1}^{\mathrm{G1}}\cdot\mathrm{X2}^{\mathrm{G2}} \tag{184}$$

8.43 Reaction J46

This is an irreversible reaction of one reactant forming two products influenced by 19 modifiers.

Name J46

Notes Lysosomal degradation of Hsc70-asyn

Reaction equation

$$\mathrm{Hsc70\_asyn} \xrightarrow{\mathrm{Lysosome\_0,\ Hsc70\_asyn,\ Lysosome\_0,\ Hsc70\_asyn,\ Lysosome\_0,\ Hsc70\_asyn,\ Lysosome\_0,\ Hsc70\_as}} \tag{185}$$

Reactant

Table 132: Properties of each reactant.

Id	Name	SBO
Hsc70_asyn	Hsc70-asyn	

Modifiers

Table 133: Properties of each modifier.

Id	Name	SBO
Lysosome_0	Lysosome	
Hsc70_asyn	Hsc70-asyn	
Lysosome_0	Lysosome	
Hsc70_asyn	Hsc70-asyn	
Lysosome_0	Lysosome	
Hsc70_asyn	Hsc70-asyn	
Lysosome_0	Lysosome	
Hsc70_asyn	Hsc70-asyn	
Lysosome_0	Lysosome	
Hsc70_asyn	Hsc70-asyn	
Lysosome_0	Lysosome	
Hsc70_asyn	Hsc70-asyn	
Lysosome_0	Lysosome	

Id	Name	SBO
Hsc70_asyn	Hsc70-asyn	
Lysosome_0	Lysosome	
Hsc70_asyn	Hsc70-asyn	
Lysosome_0	Lysosome	
Hsc70_asyn	Hsc70-asyn	
Lysosome_0	Lysosome	

Products

Table 134: Properties of each product.

Id	Name	SBO
Hsc70	Hsc70	
Fragments	Fragments	

Kinetic Law

Derived unit contains undeclared units

$$v_{43} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J1Sub1Mod}\,(\text{k46}, [\text{Hsc70\_asyn}], \text{g4681}, [\text{Lysosome\_0}], \text{g4677}) \tag{186}$$

$$\text{J1Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \tag{187}$$

$$\text{J1Sub1Mod}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \tag{188}$$

8.44 Reaction J47

This is an irreversible reaction of one reactant forming two products influenced by 19 modifiers.

Name J47

Notes Lysosomal degradation of Hsc70-protofibril

Reaction equation

$$\text{Hsc70\_Protofibril} \xrightarrow{\text{Lysosome\_0, Hsc70\_Protofibril, Lysosome\_0, Hsc70\_Protofibril, Lysosome\_0, Hsc70\_Protofibril,}} \tag{189}$$

Reactant

Table 135: Properties of each reactant.

Id	Name	SBO
Hsc70_Protofibril	Hsc70-Protofibril	

Modifiers

Table 136: Properties of each modifier.

Id	Name	SBO
Lysosome_0	Lysosome	
Hsc70_Protofibril	Hsc70-Protofibril	
Lysosome_0	Lysosome	
Hsc70_Protofibril	Hsc70-Protofibril	
Lysosome_0	Lysosome	
Hsc70_Protofibril	Hsc70-Protofibril	
Lysosome_0	Lysosome	
Hsc70_Protofibril	Hsc70-Protofibril	
Lysosome_0	Lysosome	
Hsc70_Protofibril	Hsc70-Protofibril	
Lysosome_0	Lysosome	
Hsc70_Protofibril	Hsc70-Protofibril	
Lysosome_0	Lysosome	
Hsc70_Protofibril	Hsc70-Protofibril	
Lysosome_0	Lysosome	
Hsc70_Protofibril	Hsc70-Protofibril	
Lysosome_0	Lysosome	
Hsc70_Protofibril	Hsc70-Protofibril	
Lysosome_0	Lysosome	

Products

Table 137: Properties of each product.

Id	Name	SBO
Hsc70 Fragments	Hsc70 Fragments	

Kinetic Law

Derived unit contains undeclared units

$$v_{44} = \mathrm{vol}\,(\mathrm{Neuronal\_cytosol}) \cdot \mathrm{J1Sub1Mod}\,(\mathrm{k47}, [\mathrm{Hsc70\_Protofibril}], \mathrm{g4782}, [\mathrm{Lysosome\_0}], \mathrm{g4777}) \tag{190}$$

$$\mathrm{J1Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{191}$$

$$\mathrm{J1Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{192}$$

8.45 Reaction J48

This is an irreversible reaction of one reactant forming two products influenced by 19 modifiers.

Name J48

Notes `Lysosomal degradation of Hsc70-fibril`

Reaction equation

$$\mathrm{Hsc70\_fibril} \xrightarrow{\mathrm{Lysosome\_0,\ Hsc70\_fibril,\ Lysosome\_0,\ Hsc70\_fibril,\ Lysosome\_0,\ Hsc70\_fibril,\ Lysosome\_0,\ Hsc70\_fi}} \tag{193}$$

Reactant

Table 138: Properties of each reactant.

Id	Name	SBO
`Hsc70_fibril`	Hsc70-fibril	

Modifiers

Table 139: Properties of each modifier.

Id	Name	SBO
`Lysosome_0`	Lysosome	
`Hsc70_fibril`	Hsc70-fibril	
`Lysosome_0`	Lysosome	
`Hsc70_fibril`	Hsc70-fibril	
`Lysosome_0`	Lysosome	
`Hsc70_fibril`	Hsc70-fibril	
`Lysosome_0`	Lysosome	
`Hsc70_fibril`	Hsc70-fibril	
`Lysosome_0`	Lysosome	

Id	Name	SBO
Hsc70_fibril	Hsc70-fibril	
Lysosome_0	Lysosome	
Hsc70_fibril	Hsc70-fibril	
Lysosome_0	Lysosome	
Hsc70_fibril	Hsc70-fibril	
Lysosome_0	Lysosome	
Hsc70_fibril	Hsc70-fibril	
Lysosome_0	Lysosome	
Hsc70_fibril	Hsc70-fibril	
Lysosome_0	Lysosome	

Products

Table 140: Properties of each product.

Id	Name	SBO
Hsc70	Hsc70	
Fragments	Fragments	

Kinetic Law

Derived unit contains undeclared units

$$v_{45} = \mathrm{vol}\,(\mathrm{Neuronal\_cytosol}) \cdot \mathrm{J1Sub1Mod}\,(\mathrm{k48}, [\mathrm{Hsc70\_fibril}], \mathrm{g4883}, [\mathrm{Lysosome\_0}], \mathrm{g4877}) \tag{194}$$

$$\mathrm{J1Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{195}$$

$$\mathrm{J1Sub1Mod}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{196}$$

8.46 Reaction J50

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J50

Notes `Autophagosome engulf alpha-synuclein`

Reaction equation

$$\mathrm{Alpha\_synuclein} + \mathrm{Preautophagosome\_membrane} \xrightarrow{\mathrm{Alpha\_synuclein,\ Preautophagosome\_membrane,\ Alpha\_synuclein}} \tag{197}$$

Reactants

Table 141: Properties of each reactant.

Id	Name	SBO
Alpha_synuclein	Alpha_synuclein	
Preautophagosome_membrane	Preautophagosome_membrane	

Modifiers

Table 142: Properties of each modifier.

Id	Name	SBO
Alpha_synuclein	Alpha_synuclein	
Preautophagosome_membrane	Preautophagosome_membrane	
Alpha_synuclein	Alpha_synuclein	
Preautophagosome_membrane	Preautophagosome_membrane	
Alpha_synuclein	Alpha_synuclein	
Preautophagosome_membrane	Preautophagosome_membrane	
Alpha_synuclein	Alpha_synuclein	
Preautophagosome_membrane	Preautophagosome_membrane	
Alpha_synuclein	Alpha_synuclein	
Preautophagosome_membrane	Preautophagosome_membrane	
Alpha_synuclein	Alpha_synuclein	
Preautophagosome_membrane	Preautophagosome_membrane	
Alpha_synuclein	Alpha_synuclein	
Preautophagosome_membrane	Preautophagosome_membrane	
Alpha_synuclein	Alpha_synuclein	
Preautophagosome_membrane	Preautophagosome_membrane	
Alpha_synuclein	Alpha_synuclein	
Preautophagosome_membrane	Preautophagosome_membrane	

Product

Table 143: Properties of each product.

Id	Name	SBO
Autophagosome_0	Autophagosome	

Kinetic Law

Derived unit contains undeclared units

$$v_{46} = \text{J2Sub}\left(\text{k50}, [\text{Alpha\_synuclein}], \text{g501}, [\text{Preautophagosome\_membrane}], \text{g5080}\right) \quad (198)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (199)$$

8.47 Reaction J51

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J51

Notes Autophagosome engulf protofibril

Reaction equation

$$\text{Protofibril} + \text{Preautophagosome\_membrane} \xrightarrow{\text{Protofibril, Preautophagosome\_membrane, Protofibril, Preautophagoson} \quad (200)$$

Reactants

Table 144: Properties of each reactant.

Id	Name	SBO
Protofibril	Protofibril	
Preautophagosome_membrane	Preautophagosome_membrane	

Modifiers

Table 145: Properties of each modifier.

Id	Name	SBO
Protofibril	Protofibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Protofibril	Protofibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Protofibril	Protofibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Protofibril	Protofibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Protofibril	Protofibril	

Id	Name	SBO
Preautophagosome_membrane	Preautophagosome_membrane	
Protofibril	Protofibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Protofibril	Protofibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Protofibril	Protofibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Protofibril	Protofibril	
Preautophagosome_membrane	Preautophagosome_membrane	

Product

Table 146: Properties of each product.

Id	Name	SBO
Autophagosome_0	Autophagosome	

Kinetic Law

Derived unit contains undeclared units

$$v_{47} = \text{J2Sub}\left(\text{k51}, [\text{Protofibril}], \text{g512}, [\text{Preautophagosome\_membrane}], \text{g5180}\right) \quad (201)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (202)$$

8.48 Reaction J52

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J52

Notes Autophagosome engulf fibril

Reaction equation

$$\text{Fibril} + \text{Preautophagosome\_membrane} \xrightarrow{\text{Fibril, Preautophagosome\_membrane, Fibril, Preautophagosome\_membrane,}} \quad (203)$$

Reactants

Table 147: Properties of each reactant.

Id	Name	SBO
Fibril	Fibril	
Preautophagosome_membrane	Preautophagosome_membrane	

Modifiers

Table 148: Properties of each modifier.

Id	Name	SBO
Fibril	Fibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Fibril	Fibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Fibril	Fibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Fibril	Fibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Fibril	Fibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Fibril	Fibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Fibril	Fibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Fibril	Fibril	
Preautophagosome_membrane	Preautophagosome_membrane	
Fibril	Fibril	
Preautophagosome_membrane	Preautophagosome_membrane	

Product

Table 149: Properties of each product.

Id	Name	SBO
Autophagosome_0	Autophagosome	

Kinetic Law

Derived unit contains undeclared units

$$v_{48} = \mathrm{J2Sub}\left(\mathrm{k52}, [\mathrm{Fibril}], \mathrm{g523}, [\mathrm{Preautophagosome\_membrane}], \mathrm{g5280}\right) \quad (204)$$

$$J2Sub(K, X1, G1, X2, G2) = K \cdot X1^{G1} \cdot X2^{G2} \quad (205)$$

8.49 Reaction J53

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J53

Notes `Autophagosome engulf lewy body`

Reaction equation

$$\text{Lewy\_body} + \text{Preautophagosome\_membrane} \xrightarrow{\text{Lewy\_body, Preautophagosome\_membrane, Lewy\_body, Preautophago}} \quad (206)$$

Reactants

Table 150: Properties of each reactant.

Id	Name	SBO
`Lewy_body`	Lewy_body	
`Preautophagosome_membrane`	Preautophagosome_membrane	

Modifiers

Table 151: Properties of each modifier.

Id	Name	SBO
`Lewy_body`	Lewy_body	
`Preautophagosome_membrane`	Preautophagosome_membrane	
`Lewy_body`	Lewy_body	
`Preautophagosome_membrane`	Preautophagosome_membrane	
`Lewy_body`	Lewy_body	
`Preautophagosome_membrane`	Preautophagosome_membrane	
`Lewy_body`	Lewy_body	
`Preautophagosome_membrane`	Preautophagosome_membrane	
`Lewy_body`	Lewy_body	
`Preautophagosome_membrane`	Preautophagosome_membrane	
`Lewy_body`	Lewy_body	
`Preautophagosome_membrane`	Preautophagosome_membrane	
`Lewy_body`	Lewy_body	
`Preautophagosome_membrane`	Preautophagosome_membrane	
`Lewy_body`	Lewy_body	

Id	Name	SBO
Preautophagosome_membrane	Preautophagosome_membrane	
Lewy_body	Lewy_body	
Preautophagosome_membrane	Preautophagosome_membrane	

Product

Table 152: Properties of each product.

Id	Name	SBO
Autophagosome_0	Autophagosome	

Kinetic Law

Derived unit contains undeclared units

$$v_{49} = \text{J2Sub}\left(\text{k53}, [\text{Lewy\_body}], \text{g534}, [\text{Preautophagosome\_membrane}], \text{g5380}\right) \quad (207)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (208)$$

8.50 Reaction J54

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J54

Notes DA-S-Parkin formation

Reaction equation

$$\text{DA\_quinone} + \text{Parkin} \xrightarrow{\text{DA\_quinone, Parkin, DA\_quinone, Parkin, DA\_quinone, Parkin, DA\_quinone, Parkin, DA\_qui}} \quad (209)$$

Reactants

Table 153: Properties of each reactant.

Id	Name	SBO
DA_quinone	DA_quinone	
Parkin	Parkin	

Modifiers

Table 154: Properties of each modifier.

Id	Name	SBO
DA_quinone	DA_quinone	
Parkin	Parkin	
DA_quinone	DA_quinone	
Parkin	Parkin	
DA_quinone	DA_quinone	
Parkin	Parkin	
DA_quinone	DA_quinone	
Parkin	Parkin	
DA_quinone	DA_quinone	
Parkin	Parkin	
DA_quinone	DA_quinone	
Parkin	Parkin	
DA_quinone	DA_quinone	
Parkin	Parkin	
DA_quinone	DA_quinone	
Parkin	Parkin	
DA_quinone	DA_quinone	
Parkin	Parkin	

Product

Table 155: Properties of each product.

Id	Name	SBO
DA_S_parkin	DA-S-parkin	

Kinetic Law

Derived unit contains undeclared units

$$v_{50} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k54}, [\mathrm{DA\_quinone}], \mathrm{g5410}, [\mathrm{Parkin}], \mathrm{g5419}\right) \quad (210)$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (211)$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (212)$$

8.51 Reaction J55

This is an irreversible reaction of two reactants forming two products influenced by 18 modifiers.

Name J55

Notes `DA-quinone synthesis from DA and superoxide`

Reaction equation

$$\text{Dopamine} + \text{O2} \xrightarrow{\text{Dopamine, O2, Dopamine, O2, Dopamine, O2, Dopamine, O2, Dopamine, O2, Dopamine, O2, Do}} \tag{213}$$

Reactants

Table 156: Properties of each reactant.

Id	Name	SBO
`Dopamine`	Dopamine	
`O2`	O2-	

Modifiers

Table 157: Properties of each modifier.

Id	Name	SBO
`Dopamine`	Dopamine	
`O2`	O2-	
`Dopamine`	Dopamine	
`O2`	O2-	
`Dopamine`	Dopamine	
`O2`	O2-	
`Dopamine`	Dopamine	
`O2`	O2-	
`Dopamine`	Dopamine	
`O2`	O2-	
`Dopamine`	Dopamine	
`O2`	O2-	
`Dopamine`	Dopamine	
`O2`	O2-	
`Dopamine`	Dopamine	
`O2`	O2-	
`Dopamine`	Dopamine	

Id	Name	SBO
O2	O2-	

Products

Table 158: Properties of each product.

Id	Name	SBO
H2O2	H2O2	
DA_quinone	DA_quinone	

Kinetic Law

Derived unit contains undeclared units

$$v_{51} = \text{vol}\,(\text{Neuronal\_cytosol}) \cdot \text{J2Sub}\,(\text{k55}, [\text{Dopamine}], \text{g556}, [\text{O2}], \text{g5586}) \tag{214}$$

$$\text{J2Sub}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \tag{215}$$

$$\text{J2Sub}\,(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \tag{216}$$

8.52 Reaction J56

This is an irreversible reaction of one reactant forming two products influenced by 19 modifiers.

Name J56

Notes Superoxide dismutase reaction

Reaction equation

$$\text{O2} \xrightarrow{\text{SOD, O2, SOD, O2, SOD, O2, SOD, O2, SOD, O2, SOD, O2, SOD, O2, SOD, O2, SOD, O2, SOD}} \text{H2O2} + \text{O} \tag{217}$$

Reactant

Table 159: Properties of each reactant.

Id	Name	SBO
O2	O2-	

Modifiers

Table 160: Properties of each modifier.

Id	Name	SBO
SOD	SOD	
O2	O2-	
SOD	SOD	
O2	O2-	
SOD	SOD	
O2	O2-	
SOD	SOD	
O2	O2-	
SOD	SOD	
O2	O2-	
SOD	SOD	
O2	O2-	
SOD	SOD	
O2	O2-	
SOD	SOD	
O2	O2-	
SOD	SOD	
O2	O2-	
SOD	SOD	

Products

Table 161: Properties of each product.

Id	Name	SBO
H2O2	H2O2	
O2_0	O2	

Kinetic Law

Derived unit contains undeclared units

$$v_{52} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J1Sub1Mod}\left(\mathrm{k56}, [\mathrm{O2}], \mathrm{g5686}, [\mathrm{SOD}], \mathrm{g5687}\right) \quad (218)$$

$$\mathrm{J1Sub1Mod}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (219)$$

$$\mathrm{J1Sub1Mod}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \quad (220)$$

8.53 Reaction J57

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J57

Notes DA-GSH formation

Reaction equation

$$\text{DA\_quinone} + \text{GSH} \xrightarrow{\text{DA\_quinone, GSH, DA\_quinone, GSH, DA\_quinone, GSH, DA\_quinone, GSH, DA\_quinone, C}} \tag{221}$$

Reactants

Table 162: Properties of each reactant.

Id	Name	SBO
DA_quinone	DA_quinone	
GSH	GSH	

Modifiers

Table 163: Properties of each modifier.

Id	Name	SBO
DA_quinone	DA_quinone	
GSH	GSH	
DA_quinone	DA_quinone	
GSH	GSH	
DA_quinone	DA_quinone	
GSH	GSH	
DA_quinone	DA_quinone	
GSH	GSH	
DA_quinone	DA_quinone	
GSH	GSH	
DA_quinone	DA_quinone	
GSH	GSH	
DA_quinone	DA_quinone	
GSH	GSH	
DA_quinone	DA_quinone	
GSH	GSH	
DA_quinone	DA_quinone	

Id	Name	SBO
GSH	GSH	

Product

Table 164: Properties of each product.

Id	Name	SBO
DA_GSH	DA-GSH	

Kinetic Law

Derived unit contains undeclared units

$$v_{53} = \text{vol}\left(\text{Neuronal\_cytosol}\right) \cdot \text{J2Sub}\left(\text{k57}, [\text{DA\_quinone}], \text{g5710}, [\text{GSH}], \text{g5762}\right) \quad (222)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (223)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (224)$$

8.54 Reaction J100

This is an irreversible reaction of three reactants forming three products influenced by 27 modifiers.

Name J100

Notes Neuromelanin synthesis from L-DOPA

Reaction equation

$$\text{L\_Dopa} + \text{O2\_0} + \text{Cysteine} \xrightarrow{\text{L\_Dopa, O2\_0, Cysteine, L\_Dopa, O2\_0, Cysteine, L\_Dopa, O2\_0, Cysteine, L\_Dopa, O}} \quad (225)$$

Reactants

Table 165: Properties of each reactant.

Id	Name	SBO
L_Dopa	L-Dopa	
O2_0	O2	
Cysteine	Cysteine	

Modifiers

Table 166: Properties of each modifier.

Id	Name	SBO
L_Dopa	L-Dopa	
O2_0	O2	
Cysteine	Cysteine	
L_Dopa	L-Dopa	
O2_0	O2	
Cysteine	Cysteine	
L_Dopa	L-Dopa	
O2_0	O2	
Cysteine	Cysteine	
L_Dopa	L-Dopa	
O2_0	O2	
Cysteine	Cysteine	
L_Dopa	L-Dopa	
O2_0	O2	
Cysteine	Cysteine	
L_Dopa	L-Dopa	
O2_0	O2	
Cysteine	Cysteine	
L_Dopa	L-Dopa	
O2_0	O2	
Cysteine	Cysteine	
L_Dopa	L-Dopa	
O2_0	O2	
Cysteine	Cysteine	
L_Dopa	L-Dopa	
O2_0	O2	
Cysteine	Cysteine	

Products

Table 167: Properties of each product.

Id	Name	SBO
Neuromelanin	Neuromelanin	
H2O2	H2O2	
CO2	CO2	

Kinetic Law

Derived unit contains undeclared units

$$v_{54} = \mathrm{vol}\,(\mathrm{Neuronal\_cytosol}) \cdot \mathrm{J3Sub}\,(\mathrm{k100}, [\mathrm{L\_Dopa}], \mathrm{g10037}, [\mathrm{O2\_0}], \mathrm{g10051}, [\mathrm{Cysteine}], \mathrm{g100115}) \quad (226)$$

$$\mathrm{J3Sub}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \quad (227)$$

$$\mathrm{J3Sub}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \quad (228)$$

8.55 Reaction J101

This is an irreversible reaction of three reactants forming three products influenced by 27 modifiers.

Name J101

Notes `Neuromelanin synthesis from L-Tyr`

Reaction equation

$$\mathrm{L\_Tyr} + \mathrm{O2\_0} + \mathrm{Cysteine} \xrightarrow{\mathrm{L\_Tyr},\ \mathrm{O2\_0},\ \mathrm{Cysteine},\ \mathrm{L\_Tyr},\ \mathrm{O2\_0},\ \mathrm{Cysteine},\ \mathrm{L\_Tyr},\ \mathrm{O2\_0},\ \mathrm{Cysteine},\ \mathrm{L\_Tyr},\ \mathrm{O2\_0},\ \mathrm{Cyste}} \quad (229)$$

Reactants

Table 168: Properties of each reactant.

Id	Name	SBO
`L_Tyr`	L-Tyr	
`O2_0`	O2	
`Cysteine`	Cysteine	

Modifiers

Table 169: Properties of each modifier.

Id	Name	SBO
`L_Tyr`	L-Tyr	
`O2_0`	O2	
`Cysteine`	Cysteine	

Id	Name	SBO
L_Tyr	L-Tyr	
O2_0	O2	
Cysteine	Cysteine	
L_Tyr	L-Tyr	
O2_0	O2	
Cysteine	Cysteine	
L_Tyr	L-Tyr	
O2_0	O2	
Cysteine	Cysteine	
L_Tyr	L-Tyr	
O2_0	O2	
Cysteine	Cysteine	
L_Tyr	L-Tyr	
O2_0	O2	
Cysteine	Cysteine	
L_Tyr	L-Tyr	
O2_0	O2	
Cysteine	Cysteine	
L_Tyr	L-Tyr	
O2_0	O2	
Cysteine	Cysteine	
L_Tyr	L-Tyr	
O2_0	O2	
Cysteine	Cysteine	

Products

Table 170: Properties of each product.

Id	Name	SBO
Neuromelanin	Neuromelanin	
H2O2	H2O2	
CO2	CO2	

Kinetic Law

Derived unit contains undeclared units

$$v_{55} = \text{vol}\left(\text{Neuronal\_cytosol}\right) \cdot \text{J3Sub}\left(\text{k101}, [\text{L\_Tyr}], \text{g10136}, [\text{O2\_0}], \text{g10151}, [\text{Cysteine}], \text{g101115}\right) \quad (230)$$

$$\mathrm{J3Sub}\left(\mathrm{K},\mathrm{X1},\mathrm{G1},\mathrm{X2},\mathrm{G2},\mathrm{X3},\mathrm{G3}\right) = \mathrm{K}\cdot\mathrm{X1}^{\mathrm{G1}}\cdot\mathrm{X2}^{\mathrm{G2}}\cdot\mathrm{X3}^{\mathrm{G3}} \tag{231}$$

$$\mathrm{J3Sub}\left(\mathrm{K},\mathrm{X1},\mathrm{G1},\mathrm{X2},\mathrm{G2},\mathrm{X3},\mathrm{G3}\right) = \mathrm{K}\cdot\mathrm{X1}^{\mathrm{G1}}\cdot\mathrm{X2}^{\mathrm{G2}}\cdot\mathrm{X3}^{\mathrm{G3}} \tag{232}$$

8.56 Reaction J102

This is an irreversible reaction of three reactants forming two products influenced by 27 modifiers.

Name J102

Notes Neuromelanin synthesis from DA quinone

Reaction equation

$$\mathrm{DA\_quinone} + \mathrm{O2\_0} + \mathrm{Cysteine} \xrightarrow{\mathrm{DA\_quinone,\ O2\_0,\ Cysteine,\ DA\_quinone,\ O2\_0,\ Cysteine,\ DA\_quinone,\ O2\_0,\ Cy}} \tag{233}$$

Reactants

Table 171: Properties of each reactant.

Id	Name	SBO
DA_quinone	DA_quinone	
O2_0	O2	
Cysteine	Cysteine	

Modifiers

Table 172: Properties of each modifier.

Id	Name	SBO
DA_quinone	DA_quinone	
O2_0	O2	
Cysteine	Cysteine	
DA_quinone	DA_quinone	
O2_0	O2	
Cysteine	Cysteine	
DA_quinone	DA_quinone	
O2_0	O2	
Cysteine	Cysteine	
DA_quinone	DA_quinone	

Id	Name	SBO
O2_0	O2	
Cysteine	Cysteine	
DA_quinone	DA_quinone	
O2_0	O2	
Cysteine	Cysteine	
DA_quinone	DA_quinone	
O2_0	O2	
Cysteine	Cysteine	
DA_quinone	DA_quinone	
O2_0	O2	
Cysteine	Cysteine	
DA_quinone	DA_quinone	
O2_0	O2	
Cysteine	Cysteine	
DA_quinone	DA_quinone	
O2_0	O2	
Cysteine	Cysteine	

Products

Table 173: Properties of each product.

Id	Name	SBO
Neuromelanin	Neuromelanin	
CO2	CO2	

Kinetic Law

Derived unit contains undeclared units

$$v_{56} = \mathrm{vol}\,(\mathrm{Neuronal\_cytosol}) \cdot \mathrm{J3Sub}\,(\mathrm{k102}, [\mathrm{DA\_quinone}], \mathrm{g10210}, [\mathrm{O2\_0}], \mathrm{g10251}, [\mathrm{Cysteine}], \mathrm{g102115}) \tag{234}$$

$$\mathrm{J3Sub}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \tag{235}$$

$$\mathrm{J3Sub}\,(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}, \mathrm{X3}, \mathrm{G3}) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \cdot \mathrm{X3}^{\mathrm{G3}} \tag{236}$$

8.57 Reaction J115

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J115

Notes Neuromelanin Fe3+ sequestration

Reaction equation

$$\mathrm{Fe3} + \mathrm{Neuromelanin} \xrightarrow{\text{Fe3, Neuromelanin, Fe3, Neuromelanin, Fe3, Neuromelanin, Fe3, Neuromelanin, Fe3, Neuron}} \tag{237}$$

Reactants

Table 174: Properties of each reactant.

Id	Name	SBO
Fe3	Fe3+	
Neuromelanin	Neuromelanin	

Modifiers

Table 175: Properties of each modifier.

Id	Name	SBO
Fe3	Fe3+	
Neuromelanin	Neuromelanin	
Fe3	Fe3+	
Neuromelanin	Neuromelanin	
Fe3	Fe3+	
Neuromelanin	Neuromelanin	
Fe3	Fe3+	
Neuromelanin	Neuromelanin	
Fe3	Fe3+	
Neuromelanin	Neuromelanin	
Fe3	Fe3+	
Neuromelanin	Neuromelanin	
Fe3	Fe3+	
Neuromelanin	Neuromelanin	
Fe3	Fe3+	
Neuromelanin	Neuromelanin	
Fe3	Fe3+	

Id	Name	SBO
Neuromelanin	Neuromelanin	

Product

Table 176: Properties of each product.

Id	Name	SBO
Neuromelanin_ntox_Fe3	Neuromelanin-ntox-Fe3+	

Kinetic Law

Derived unit contains undeclared units

$$v_{57} = \text{vol}\left(\text{Neuronal\_cytosol}\right) \cdot \text{J2Sub}\left(\text{k115}, [\text{Fe3}], \text{g11565}, [\text{Neuromelanin}], \text{g115118}\right) \quad (238)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (239)$$

$$\text{J2Sub}\left(\text{K}, \text{X1}, \text{G1}, \text{X2}, \text{G2}\right) = \text{K} \cdot \text{X1}^{\text{G1}} \cdot \text{X2}^{\text{G2}} \quad (240)$$

8.58 Reaction J116

This is an irreversible reaction of two reactants forming one product influenced by 18 modifiers.

Name J116

Notes Neuromelanin neurotoxin sequestration

Reaction equation

$$\text{Neuromelanin} + \text{Neurotoxins} \xrightarrow{\text{Neuromelanin, Neurotoxins, Neuromelanin, Neurotoxins, Neuromelanin, Neurotoxins}} \quad (241)$$

Reactants

Table 177: Properties of each reactant.

Id	Name	SBO
Neuromelanin	Neuromelanin	
Neurotoxins	Neurotoxins	

Modifiers

Table 178: Properties of each modifier.

Id	Name	SBO
Neuromelanin	Neuromelanin	
Neurotoxins	Neurotoxins	
Neuromelanin	Neuromelanin	
Neurotoxins	Neurotoxins	
Neuromelanin	Neuromelanin	
Neurotoxins	Neurotoxins	
Neuromelanin	Neuromelanin	
Neurotoxins	Neurotoxins	
Neuromelanin	Neuromelanin	
Neurotoxins	Neurotoxins	
Neuromelanin	Neuromelanin	
Neurotoxins	Neurotoxins	
Neuromelanin	Neuromelanin	
Neurotoxins	Neurotoxins	
Neuromelanin	Neuromelanin	
Neurotoxins	Neurotoxins	
Neuromelanin	Neuromelanin	
Neurotoxins	Neurotoxins	

Product

Table 179: Properties of each product.

Id	Name	SBO
Neuromelanin_ntox_Fe3	Neuromelanin-ntox-Fe3+	

Kinetic Law

Derived unit contains undeclared units

$$v_{58} = \mathrm{vol}\left(\mathrm{Neuronal\_cytosol}\right) \cdot \mathrm{J2Sub}\left(\mathrm{k116}, [\mathrm{Neuromelanin}], \mathrm{g116118}, [\mathrm{Neurotoxins}], \mathrm{g11642}\right) \tag{242}$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{243}$$

$$\mathrm{J2Sub}\left(\mathrm{K}, \mathrm{X1}, \mathrm{G1}, \mathrm{X2}, \mathrm{G2}\right) = \mathrm{K} \cdot \mathrm{X1}^{\mathrm{G1}} \cdot \mathrm{X2}^{\mathrm{G2}} \tag{244}$$

9 Derived Rate Equations

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

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

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

9.1 Species `Protofibril`

Name Protofibril

Notes `Alpha synuclein protofibril`

Initial concentration $0.05\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in 52 reactions (as a reactant in J2, J33, J35, J44, J51 and as a product in J1, J32 and as a modifier in J2, J2, J2, J2, J2, J2, J2, J2, J2, J33, J33, J33, J33, J33, J33, J33, J33, J33, J35, J35, J35, J35, J35, J35, J35, J35, J35, J44, J44, J44, J44, J44, J44, J44, J44, J44, J51, J51, J51, J51, J51, J51, J51, J51, J51).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Protofibril} = v_1 + v_{33} - v_2 - v_{34} - v_{36} - v_{41} - v_{47} \tag{245}$$

9.2 Species `Fibril`

Name Fibril

Notes `Alpha synuclein fibril`

Initial concentration $0.025\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in 32 reactions (as a reactant in J3, J45, J52 and as a product in J2, J35 and as a modifier in J3, J3, J3, J3, J3, J3, J3, J3, J3, J45, J45, J45, J45, J45, J45, J45, J45, J45, J52, J52, J52, J52, J52, J52, J52, J52, J52).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Fibril} = v_2 + v_{36} - v_3 - v_{42} - v_{48} \tag{246}$$

9.3 Species Lewy_body

Name Lewy_body

Notes Lewy Bodies

Initial concentration 0.01 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J53 and as a product in J3 and as a modifier in J53, J53, J53, J53, J53, J53, J53, J53, J53).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Lewy\_body} = v_3 - v_{49} \tag{247}$$

9.4 Species Dopamine

Name Dopamine

Notes Dopamine

Initial concentration 2 dimensionless · dimensionless^{-1}

This species takes part in 41 reactions (as a reactant in J15, J18, J19, J55 and as a product in J14 and as a modifier in J15, J15, J15, J15, J15, J15, J15, J15, J15, J18, J18, J18, J18, J18, J18, J18, J18, J18, J19, J19, J19, J19, J19, J19, J19, J19, J19, J55, J55, J55, J55, J55, J55, J55, J55, J55, J55).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Dopamine} = v_{12} - v_{13} - v_{16} - v_{17} - v_{51} \tag{248}$$

9.5 Species OH

Name OH-

Notes Hydroxide

Initial concentration 0.5 dimensionless · dimensionless^{-1}

This species takes part in one reaction (as a product in J20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{OH} = v_{18} \tag{249}$$

9.6 Species OH_radical

Name OH_radical

Notes Hydroxyl radical

Initial concentration 0.02 dimensionless · dimensionless^{-1}

This species takes part in one reaction (as a product in J20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{OH\_radical} = v_{18} \tag{250}$$

9.7 Species H2O2

Name H2O2

Notes Hidrogen Peroxide

Initial concentration 0.1 dimensionless · dimensionless^{-1}

This species takes part in 35 reactions (as a reactant in J20, J22, J23 and as a product in J19, J55, J56, J100, J101 and as a modifier in J20, J20, J20, J20, J20, J20, J20, J20, J20, J22, J22, J22, J22, J22, J22, J22, J22, J23, J23, J23, J23, J23, J23, J23, J23, J23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H2O2} = v_{17} + v_{51} + v_{52} + v_{54} + v_{55} - v_{18} - v_{20} - v_{21} \tag{251}$$

9.8 Species DA_quinone

Name DA_quinone

Notes Dopamine quinone (oxidized form)

Initial concentration 0.05 dimensionless · dimensionless^{-1}

This species takes part in 32 reactions (as a reactant in J54, J57, J102 and as a product in J18, J55 and as a modifier in J54, J54, J54, J54, J54, J54, J54, J54, J54, J57, J57, J57, J57, J57, J57, J57, J57, J57, J102, J102, J102, J102, J102, J102, J102, J102, J102).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DA\_quinone} = v_{16} + v_{51} - v_{50} - v_{53} - v_{56} \tag{252}$$

9.9 Species Ubiquitin

Name Ubiquitin

Notes Ubiquitin

Initial concentration 1 dimensionless · dimensionless^{-1}

This species takes part in 15 reactions (as a reactant in J6 and as a product in J4, J26r, J27r, J28r, J38 and as a modifier in J6, J6, J6, J6, J6, J6, J6, J6, J6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ubiquitin} = 4\,v_4 + 2\,v_{25} + 3\,v_{27} + 4\,v_{29} + 4\,v_{39} - v_5 \tag{253}$$

9.10 Species E1

Name E1

Notes Ubiquitin-activating enzymes (E1)

Initial concentration 0.2 dimensionless · dimensionless^{-1}

This species takes part in 15 reactions (as a reactant in J6 and as a product in J7, J26f, J27f, J28f, J29 and as a modifier in J6, J6, J6, J6, J6, J6, J6, J6, J6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E1} = v_6 + v_{24} + v_{26} + v_{28} + v_{30} - v_5 \tag{254}$$

9.11 Species Ub_E1

Name Ub-E1

Notes Ubiquitin - Ubiquitin-activating enzymes (E1)

Initial concentration 0.35 dimensionless · dimensionless^{-1}

This species takes part in 51 reactions (as a reactant in J7, J26f, J27f, J28f, J29 and as a product in J6 and as a modifier in J7, J7, J7, J7, J7, J7, J7, J7, J7, J26f, J26f, J26f, J26f, J26f, J26f, J26f, J26f, J27f, J27f, J27f, J27f, J27f, J27f, J27f, J27f, J27f, J28f, J28f, J28f, J28f, J28f, J28f, J28f, J28f, J28f, J29, J29, J29, J29, J29, J29, J29, J29, J29).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ub\_E1} = v_5 - v_6 - v_{24} - v_{26} - v_{28} - v_{30} \tag{255}$$

9.12 Species UbcH8

Name UbcH8

Notes Ubiquitin/ISG15-conjugating enzyme E2

Initial concentration 0.2 dimensionless · dimensionless^{-1}

This species takes part in 15 reactions (as a reactant in J7 and as a product in J11, J26r, J27r, J28r, J37 and as a modifier in J7, J7, J7, J7, J7, J7, J7, J7, J7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UbcH8} = v_{10} + v_{25} + v_{27} + v_{29} + v_{38} - v_6 \tag{256}$$

9.13 Species UbcH8_Ub

Name UbcH8-Ub

Notes Ubiquitin - Ubiquitin/ISG15-conjugating enzyme E2

Initial concentration 0.35 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J26f and as a product in J7 and as a modifier in J26f, J26f, J26f, J26f, J26f, J26f, J26f, J26f, J26f).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UbcH8\_Ub} = v_6 - v_{24} \tag{257}$$

9.14 Species Parkin

Name Parkin

Notes E3 ubiquitin-protein ligase parkin

Initial concentration 0.2 dimensionless · dimensionless^{-1}

This species takes part in 31 reactions (as a reactant in J8, J9, J54 and as a product in J4 and as a modifier in J8, J8, J8, J8, J8, J8, J8, J8, J8, J9, J9, J9, J9, J9, J9, J9, J9, J9, J54, J54, J54, J54, J54, J54, J54, J54, J54, J54).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Parkin} = v_4 - v_7 - v_8 - v_{50} \tag{258}$$

9.15 Species Parkin_sub

Name Parkin-sub

Notes E3 ubiquitin-protein ligase parkin - Substrate

Initial concentration 0.1 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J11 and as a product in J8 and as a modifier in J11, J11, J11, J11, J11, J11, J11, J11, J11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Parkin\_sub} = v_7 - v_{10} \tag{259}$$

9.16 Species Parkin_synphilin_1

Name Parkin-synphilin-1

Notes E3 ubiquitin-protein ligase parkin - synphilin-1 complex

Initial concentration 1.3 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J10 and as a product in J9 and as a modifier in J10, J10, J10, J10, J10, J10, J10, J10, J10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Parkin\_synphilin\_1} = v_8 - v_9 \tag{260}$$

9.17 Species Parkin_synphilin_1_ub

Name Parkin-synphilin-1-ub

Notes E3 ubiquitin-protein ligase parkin - synphilin-1-ubiquitin complex

Initial concentration 2.5 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J3 and as a product in J10 and as a modifier in J3, J3, J3, J3, J3, J3, J3, J3, J3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Parkin\_synphilin\_1\_ub} = v_9 - v_3 \tag{261}$$

9.18 Species Parkin_sub_ub4

Name Parkin-sub-ub4

Notes E3 ubiquitin-protein ligase parkin - 4 Ubiquitinated substrate

Initial concentration 0.2 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J4 and as a product in J11 and as a modifier in J4, J4, J4, J4, J4, J4, J4, J4, J4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Parkin\_sub\_ub4} = v_{10} - v_4 \tag{262}$$

9.19 Species Fragments

Name Fragments

Notes Degraded fragments

Initial concentration 0.1 dimensionless · dimensionless^{-1}

This species takes part in six reactions (as a product in J4, J36, J38, J46, J47, J48).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Fragments} = v_4 + v_{37} + v_{39} + v_{43} + v_{44} + v_{45} \tag{263}$$

9.20 Species UCH_L1

Name UCH-L1

Notes `Ubiquitin carboxyl-terminal hydrolase isozyme L1 (UCH-L1)`

Initial concentration 0.5 dimensionless · dimensionless^{-1}

This species takes part in 73 reactions (as a reactant in J30, J33 and as a product in J31, J34, J38 and as a modifier in J4, J4, J4, J4, J4, J4, J4, J4, J4, J4, J26r, J26r, J26r, J26r, J26r, J26r, J26r, J26r, J26r, J26r, J27r, J27r, J27r, J27r, J27r, J27r, J27r, J27r, J27r, J28r, J28r, J28r, J28r, J28r, J28r, J28r, J28r, J28r, J28r, J30, J30, J30, J30, J30, J30, J30, J30, J30, J33, J33, J33, J33, J33, J33, J33, J33, J33, J38, J38, J38, J38, J38, J38, J38, J38, J38, J38).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UCH\_L1} = v_{32} + v_{35} + v_{39} - v_{31} - v_{34} \tag{264}$$

9.21 Species L_Dopa

Name L-Dopa

Notes `L-3,4-dihydroxyphenylalanine`

Initial concentration 1 dimensionless · dimensionless^{-1}

This species takes part in 21 reactions (as a reactant in J14, J100 and as a product in J13 and as a modifier in J14, J14, J14, J14, J14, J14, J14, J14, J14, J100, J100, J100, J100, J100, J100, J100, J100, J100, J100).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{L\_Dopa} = v_{11} - v_{12} - v_{54} \tag{265}$$

9.22 Species DOPAL

Name DOPAL

Notes `3,4-Dihydroxyphenylacetaldehyde (DOPAL)`

Initial concentration 0.05 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J25 and as a product in J19 and as a modifier in J25, J25, J25, J25, J25, J25, J25, J25, J25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DOPAL} = v_{17} - v_{23} \tag{266}$$

9.23 Species DOPAC

Name DOPAC

Notes 3,4-Dihydroxyphenylacetic acid (DOPAC)

Initial concentration 0.3 dimensionless · dimensionless^{-1}

This species takes part in one reaction (as a product in J25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DOPAC} = v_{23} \tag{267}$$

9.24 Species GSH

Name GSH

Notes Glutathione (GSH)

Initial concentration 1.5 dimensionless · dimensionless^{-1}

This species takes part in 21 reactions (as a reactant in J23, J57 and as a product in J24 and as a modifier in J23, J23, J23, J23, J23, J23, J23, J23, J23, J57, J57, J57, J57, J57, J57, J57, J57, J57).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GSH} = v_{22} - v_{21} - v_{53} \tag{268}$$

9.25 Species GSSG

Name GSSG

Notes Glutathione disulfide (GSSG)

Initial concentration 1.5 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J24 and as a product in J23 and as a modifier in J24, J24, J24, J24, J24, J24, J24, J24, J24).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GSSG} = v_{21} - v_{22} \tag{269}$$

9.26 Species Fe2

Name Fe2+

Notes Iron (2+)

Initial concentration 0.5 dimensionless · dimensionless^{-1}

Involved in rule Fe2

This species takes part in eleven reactions (as a reactant in J20 and as a product in J21 and as a modifier in J20, J20, J20, J20, J20, J20, J20, J20, J20). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.27 Species Fe3

Name Fe3+

Notes Iron (Fe3+)

Initial concentration 0.5 dimensionless · dimensionless^{-1}

This species takes part in 21 reactions (as a reactant in J21, J115 and as a product in J20 and as a modifier in J21, J21, J21, J21, J21, J21, J21, J21, J21, J115, J115, J115, J115, J115, J115, J115, J115, J115).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fe3} = v_{18} - v_{19} - v_{57} \tag{270}$$

9.28 Species UbcH8ub2

Name UbcH8ub2

Notes 2 Ubiquitin - Ubiquitin/ISG15-conjugating enzyme E2

Initial concentration 0.35 dimensionless · dimensionless^{-1}

This species takes part in 21 reactions (as a reactant in J26r, J27f and as a product in J26f and as a modifier in J26r, J26r, J26r, J26r, J26r, J26r, J26r, J26r, J26r, J27f, J27f, J27f, J27f, J27f, J27f, J27f, J27f, J27f, J27f).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UbcH8ub2} = v_{24} - v_{25} - v_{26} \tag{271}$$

9.29 Species UbcH8ub3

Name UbcH8ub3

Notes 3 Ubiquitin - Ubiquitin/ISG15-conjugating enzyme E2

Initial concentration 0.35 dimensionless · dimensionless^{-1}

This species takes part in 21 reactions (as a reactant in J27r, J28f and as a product in J27f and as a modifier in J27r, J27r, J27r, J27r, J27r, J27r, J27r, J27r, J27r, J28f, J28f, J28f, J28f, J28f, J28f, J28f, J28f, J28f, J28f).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UbcH8ub3} = v_{26} - v_{27} - v_{28} \tag{272}$$

9.30 Species UbcH8ub4

Name UbcH8ub4

Notes 4 Ubiquitin - Ubiquitin/ISG15-conjugating enzyme E2

Initial concentration 0.35 dimensionless · dimensionless^{-1}

This species takes part in 31 reactions (as a reactant in J11, J28r, J37 and as a product in J28f and as a modifier in J11, J11, J11, J11, J11, J11, J11, J11, J11, J28r, J28r, J28r, J28r, J28r, J28r, J28r, J28r, J28r, J37, J37, J37, J37, J37, J37, J37, J37, J37).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UbcH8ub4} = v_{28} - v_{10} - v_{29} - v_{38} \tag{273}$$

9.31 Species UbcH13_Uev1a

Name UbcH13/Uev1a

Notes Ubiquitin-conjugating enzyme (E2) / Ubiquitin-conjugating enzyme (Uev1a)

Initial concentration 0.2 dimensionless · dimensionless^{-1}

This species takes part in 13 reactions (as a reactant in J29 and as a product in J10, J31, J34 and as a modifier in J29, J29, J29, J29, J29, J29, J29, J29, J29).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UbcH13\_Uev1a} = v_{9} + v_{32} + v_{35} - v_{30} \tag{274}$$

9.32 Species UbcH13_Uev1a_ub

Name UbcH13/Uev1a-ub

Notes Ubiquitin - Ubiquitin-conjugating enzyme (E2) / Ubiquitin-conjugating enzyme (Uev1a

Initial concentration 0.35 dimensionless · dimensionless^{-1}

This species takes part in 31 reactions (as a reactant in J10, J31, J34 and as a product in J29 and as a modifier in J10, J10, J10, J10, J10, J10, J10, J10, J10, J31, J31, J31, J31, J31, J31, J31, J31, J31, J34, J34, J34, J34, J34, J34, J34, J34, J34).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UbcH13\_Uev1a\_ub} = v_{30} - v_{9} - v_{32} - v_{35} \tag{275}$$

9.33 Species asyn_UCH_L1

Name asyn-UCH-L1

Notes `Alpha synuclein - Ubiquitin carboxyl-terminal hydrolase isozyme L1 (UCH-L1)`

Initial concentration $0.1\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in 21 reactions (as a reactant in J31, J37 and as a product in J30 and as a modifier in J31, J31, J31, J31, J31, J31, J31, J31, J31, J37, J37, J37, J37, J37, J37, J37, J37, J37).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{asyn\_UCH\_L1} = v_{31} - v_{32} - v_{38} \tag{276}$$

9.34 Species asyn_ub

Name asyn-ub

Notes `Ubiquitinated alpha synuclein`

Initial concentration $0.05\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in eleven reactions (as a reactant in J32 and as a product in J31 and as a modifier in J32, J32, J32, J32, J32, J32, J32, J32, J32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{asyn\_ub} = v_{32} - v_{33} \tag{277}$$

9.35 Species Protofibril_UCH_L1

Name Protofibril-UCH-L1

Notes `Alpha synuclein protofibril - Ubiquitin carboxyl-terminal hydrolase isozyme L1 (UCH`

Initial concentration $0.025\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in eleven reactions (as a reactant in J34 and as a product in J33 and as a modifier in J34, J34, J34, J34, J34, J34, J34, J34, J34).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Protofibril\_UCH\_L1} = v_{34} - v_{35} \tag{278}$$

9.36 Species Protofibril_Ub

Name Protofibril-Ub

Notes Ubiquitinated alpha synuclein protofibril

Initial concentration 0.013 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J35 and as a product in J34 and as a modifier in J35, J35, J35, J35, J35, J35, J35, J35, J35).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Protofibril\_Ub} = v_{35} - v_{36} \tag{279}$$

9.37 Species UCH_L1_asyn_ub4

Name UCH-L1-asyn-ub4

Notes Ubiquitin carboxyl-terminal hydrolase isozyme L1 (UCH-L1) - 4 Ubiquitinated alpha s

Initial concentration 0.1 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J38 and as a product in J37 and as a modifier in J38, J38, J38, J38, J38, J38, J38, J38, J38).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{UCH\_L1\_asyn\_ub4} = v_{38} - v_{39} \tag{280}$$

9.38 Species Hsc70_asyn

Name Hsc70-asyn

Notes Alpha synuclein - Heat shock cognate 70 kDa protein (chaperone)

Initial concentration 0.1 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J46 and as a product in J43 and as a modifier in J46, J46, J46, J46, J46, J46, J46, J46, J46).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Hsc70\_asyn} = v_{40} - v_{43} \tag{281}$$

9.39 Species Hsc70_Protofibril

Name Hsc70-Protofibril

Notes Alpha synuclein protofibril - Heat shock cognate 70 kDa protein (chaperone)

Initial concentration 0.025 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J47 and as a product in J44 and as a modifier in J47, J47, J47, J47, J47, J47, J47, J47, J47).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Hsc70\_Protofibril} = v_{41} - v_{44} \tag{282}$$

9.40 Species Hsc70_fibril

Name Hsc70-fibril

Notes Alpha synuclein fibril - Heat shock cognate 70 kDa protein (chaperone)

Initial concentration 0.013 dimensionless · dimensionless^{-1}

This species takes part in eleven reactions (as a reactant in J48 and as a product in J45 and as a modifier in J48, J48, J48, J48, J48, J48, J48, J48, J48).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Hsc70\_fibril} = v_{42} - v_{45} \tag{283}$$

9.41 Species Hsc70

Name Hsc70

Notes Heat shock cognate 70 kDa protein (chaperone)

Initial concentration 0.5 dimensionless · dimensionless^{-1}

This species takes part in 33 reactions (as a reactant in J43, J44, J45 and as a product in J46, J47, J48 and as a modifier in J43, J43, J43, J43, J43, J43, J43, J43, J43, J44, J44, J44, J44, J44, J44, J44, J44, J44, J44, J45, J45, J45, J45, J45, J45, J45, J45, J45).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Hsc70} = v_{43} + v_{44} + v_{45} - v_{40} - v_{41} - v_{42} \tag{284}$$

9.42 Species DA_S_parkin

Name DA-S-parkin

Notes Dopamine quinone (oxidized form) - E3 ubiquitin-protein ligase parkin

Initial concentration 0.2 dimensionless · dimensionless^{-1}

This species takes part in one reaction (as a product in J54).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DA\_S\_parkin} = v_{50} \tag{285}$$

9.43 Species O2

Name O2-

Notes Superoxide radical (O2-)

Initial concentration 0.02 dimensionless · dimensionless^{-1}

This species takes part in 21 reactions (as a reactant in J55, J56 and as a product in J18 and as a modifier in J55, J55, J55, J55, J55, J55, J55, J55, J55, J56, J56, J56, J56, J56, J56, J56, J56, J56).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{O2} = v_{16} - v_{51} - v_{52} \tag{286}$$

9.44 Species DA_GSH

Name DA-GSH

Notes Dopamine - Glutathione (GSH)

Initial concentration $0.2\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in one reaction (as a product in J57).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DA\_GSH} = v_{53} \tag{287}$$

9.45 Species Neuromelanin

Name Neuromelanin

Notes Neuromelanin (NM)

Initial concentration $1\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in 23 reactions (as a reactant in J115, J116 and as a product in J100, J101, J102 and as a modifier in J115, J115, J115, J115, J115, J115, J115, J115, J115, J116, J116, J116, J116, J116, J116, J116, J116, J116).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Neuromelanin} = v_{54} + v_{55} + v_{56} - v_{57} - v_{58} \tag{288}$$

9.46 Species Neuromelanin_ntox_Fe3

Name Neuromelanin-ntox-Fe3+

Notes Neuromelanin (NM) with neurotoxins and Fe2+. Neurotoxins such as rotenone and MPTP

Initial concentration $0.5\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in two reactions (as a product in J115, J116).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Neuromelanin\_ntox\_Fe3} = v_{57} + v_{58} \tag{289}$$

9.47 Species Alpha_synuclein

Name Alpha_synuclein

Notes Alpha synuclein

Initial concentration $0.2\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in 50 reactions (as a reactant in J1, J30, J32, J43, J50 and as a modifier in J1, J1, J1, J1, J1, J1, J1, J1, J1, J30, J30, J30, J30, J30, J30, J30, J30, J30, J32, J32, J32, J32, J32, J32, J32, J32, J32, J32, J43, J43, J43, J43, J43, J43, J43, J43, J43, J50, J50, J50, J50, J50, J50, J50, J50, J50, J50), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Alpha\_synuclein} = 0 \tag{290}$$

9.48 Species ATP

Name ATP

Notes Adenosine triphosphate (ATP)

Initial concentration $2\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in 80 reactions (as a modifier in J4, J4, J4, J4, J4, J4, J4, J4, J4, J4, J6, J6, J6, J6, J6, J6, J6, J6, J6, J6, J7, J7, J7, J7, J7, J7, J7, J7, J7, J7, J26f, J26f, J26f, J26f, J26f, J26f, J26f, J26f, J26f, J26f, J27f, J27f, J27f, J27f, J27f, J27f, J27f, J27f, J27f, J27f, J28f, J28f, J28f, J28f, J28f, J28f, J28f, J28f, J28f, J28f, J29, J29, J29, J29, J29, J29, J29, J29, J29, J29, J38, J38, J38, J38, J38, J38, J38, J38, J38, J38), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{ATP} = 0 \tag{291}$$

9.49 Species Synphilin_1

Name Synphilin-1

Notes Synphilin-1

Initial concentration $0.05\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in ten reactions (as a reactant in J9 and as a modifier in J9, J9, J9, J9, J9, J9, J9, J9, J9), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Synphilin\_1} = 0 \tag{292}$$

9.50 Species Substrate

Name Substrate

Notes Substrate

Initial concentration $0.4\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in ten reactions (as a reactant in J8 and as a modifier in J8, J8, J8, J8, J8, J8, J8, J8, J8), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Substrate} = 0 \tag{293}$$

9.51 Species TH

Name TH

Notes Tyrosine hydroxylase (TH)

Initial concentration $0.6\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in ten reactions (as a modifier in J13, J13, J13, J13, J13, J13, J13, J13, J13, J13), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{TH} = 0 \tag{294}$$

9.52 Species L_Tyr

Name L-Tyr

Notes L-Tyrosine

Initial concentration $5\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in 20 reactions (as a reactant in J13, J101 and as a modifier in J13, J13, J13, J13, J13, J13, J13, J13, J13, J101, J101, J101, J101, J101, J101, J101, J101, J101), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{L\_Tyr} = 0 \tag{295}$$

9.53 Species CO2

Name CO2

Notes Carbon dioxide (CO2)

Initial concentration 0.5 dimensionless · dimensionless^{-1}

This species takes part in four reactions (as a product in J14, J100, J101, J102), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2} = 0 \tag{296}$$

9.54 Species Neurotoxins

Name Neurotoxins

Notes Neurotoxins such as rotenone and MPTP

Initial concentration 0.01 dimensionless · dimensionless^{-1}

This species takes part in 20 reactions (as a reactant in J17, J116 and as a modifier in J17, J17, J17, J17, J17, J17, J17, J17, J17, J116, J116, J116, J116, J116, J116, J116, J116, J116), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Neurotoxins} = 0 \tag{297}$$

9.55 Species Bioamines

Name Bioamines

Notes Biogenic amine

Initial concentration 0.1 dimensionless · dimensionless^{-1}

This species takes part in ten reactions (as a reactant in J16 and as a modifier in J16, J16, J16, J16, J16, J16, J16, J16, J16), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bioamines} = 0 \tag{298}$$

9.56 Species VMAT2

Name VMAT2

Notes vesicular monoamine transporter 2 (VMAT2)

Initial concentration $2\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in ten reactions (as a modifier in J15, J15, J15, J15, J15, J15, J15, J15, J15, J15), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{VMAT2} = 0 \tag{299}$$

9.57 Species O2_0

Name O2

Notes Oxygen (O2)

Initial concentration $2\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in 62 reactions (as a reactant in J13, J18, J19, J100, J101, J102 and as a product in J22, J56 and as a modifier in J13, J13, J13, J13, J13, J13, J13, J13, J13, J18, J18, J18, J18, J18, J18, J18, J18, J19, J19, J19, J19, J19, J19, J19, J19, J19, J100, J100, J100, J100, J100, J100, J100, J100, J101, J101, J101, J101, J101, J101, J101, J101, J101, J102, J102, J102, J102, J102, J102, J102, J102, J102), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{O2\_0} = 0 \tag{300}$$

9.58 Species MAO

Name MAO

Notes L-Monoamine oxidases (MAO)

Initial concentration $1.5\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in ten reactions (as a modifier in J19, J19, J19, J19, J19, J19, J19, J19, J19, J19), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MAO} = 0 \tag{301}$$

9.59 Species NH3

Name NH3

Notes Ammonia (NH3)

Initial concentration $0.5\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in one reaction (as a product in J19), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NH3} = 0 \tag{302}$$

9.60 Species ALDH

Name ALDH

Notes Aldehyde dehydrogenases (ALDH)

Initial concentration $1.5\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in ten reactions (as a modifier in J25, J25, J25, J25, J25, J25, J25, J25, J25, J25), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ALDH} = 0 \tag{303}$$

9.61 Species NAD

Name NAD+

Notes Nicotinamide adenine dinucleotide (oxidized)

Initial concentration $1.5\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in ten reactions (as a reactant in J25 and as a modifier in J25, J25, J25, J25, J25, J25, J25, J25, J25), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = 0 \tag{304}$$

9.62 Species NADH

Name NADH

Notes Nicotinamide adenine dinucleotide (reduced)

Initial concentration 1.5 dimensionless · dimensionless^{-1}

This species takes part in one reaction (as a product in J25), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH} = 0 \tag{305}$$

9.63 Species Catalase

Name Catalase

Notes Catalase

Initial concentration 1 dimensionless · dimensionless^{-1}

This species takes part in ten reactions (as a modifier in J22, J22, J22, J22, J22, J22, J22, J22, J22, J22), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Catalase} = 0 \tag{306}$$

9.64 Species H2O

Name H2O

Notes Water (H2O)

Initial concentration 3 dimensionless · dimensionless^{-1}

This species takes part in twelve reactions (as a reactant in J19 and as a product in J22, J23 and as a modifier in J19, J19, J19, J19, J19, J19, J19, J19, J19), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H2O} = 0 \tag{307}$$

9.65 Species Gluta_per

Name Gluta_per

Notes Glutathione peroxidase

Initial concentration 0.8 dimensionless · dimensionless^{-1}

This species takes part in ten reactions (as a modifier in J23, J23, J23, J23, J23, J23, J23, J23, J23, J23), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gluta\_per} = 0 \tag{308}$$

9.66 Species Gluta_red

Name Gluta_red

Notes Glutathione reductase

Initial concentration 0.8 dimensionless · dimensionless^{-1}

This species takes part in ten reactions (as a modifier in J24, J24, J24, J24, J24, J24, J24, J24, J24, J24), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gluta\_red} = 0 \tag{309}$$

9.67 Species DDC

Name DDC

Notes Aromatic L-amino acid decarboxylase (DDC)

Initial concentration 1.5 dimensionless · dimensionless^{-1}

This species takes part in ten reactions (as a modifier in J14, J14, J14, J14, J14, J14, J14, J14, J14, J14), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DDC} = 0 \tag{310}$$

9.68 Species Preautophagosome_membrane

Name Preautophagosome_membrane

Notes Preautophagosome membrane

Initial concentration 1 dimensionless · dimensionless^{-1}

This species takes part in 40 reactions (as a reactant in J50, J51, J52, J53 and as a modifier in J50, J50, J50, J50, J50, J50, J50, J50, J50, J51, J51, J51, J51, J51, J51, J51, J51, J51, J52, J52, J52, J52, J52, J52, J52, J52, J52, J53, J53, J53, J53, J53, J53, J53, J53, J53), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Preautophagosome\_membrane} = 0 \tag{311}$$

9.69 Species SOD

Name SOD

Notes Superoxide dismutases (SOD)

Initial concentration $0.6\ \mathrm{dimensionless} \cdot \mathrm{dimensionless}^{-1}$

This species takes part in ten reactions (as a modifier in J56, J56, J56, J56, J56, J56, J56, J56, J56, J56), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{SOD} = 0 \tag{312}$$

9.70 Species Cysteine

Name Cysteine

Notes Cysteine

Initial concentration $0.5\ \mathrm{dimensionless} \cdot \mathrm{dimensionless}^{-1}$

This species takes part in 30 reactions (as a reactant in J100, J101, J102 and as a modifier in J100, J100, J100, J100, J100, J100, J100, J100, J100, J101, J101, J101, J101, J101, J101, J101, J101, J101, J102, J102, J102, J102, J102, J102, J102, J102), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cysteine} = 0 \tag{313}$$

9.71 Species V_DA

Name V-DA

Notes Vesicular dopamine

Initial concentration $10\ \mathrm{dimensionless} \cdot \mathrm{dimensionless}^{-1}$

This species takes part in one reaction (as a product in J15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{V\_DA} = v_{13} \tag{314}$$

9.72 Species V_ntox_ba

Name V-ntox-ba

Notes Vesicular neurotoxins and bio-amines. Neurotoxins such as rotenone and MPTP.

Initial concentration 0.3 dimensionless · dimensionless^{-1}

This species takes part in two reactions (as a product in J16, J17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{V\_ntox\_ba} = v_{14} + v_{15} \tag{315}$$

9.73 Species Vesicle_0

Name Vesicle

Notes Vesicle

Initial concentration 1 dimensionless · dimensionless^{-1}

This species takes part in 30 reactions (as a reactant in J15, J16, J17 and as a modifier in J15, J15, J15, J15, J15, J15, J15, J15, J15, J16, J16, J16, J16, J16, J16, J16, J16, J16, J17, J17, J17, J17, J17, J17, J17, J17, J17), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Vesicle\_0} = 0 \tag{316}$$

9.74 Species Autophagosome_0

Name Autophagosome

Notes Autophagosome

Initial concentration 0.5 dimensionless · dimensionless^{-1}

This species takes part in 14 reactions (as a reactant in J36 and as a product in J50, J51, J52, J53 and as a modifier in J36, J36, J36, J36, J36, J36, J36, J36, J36).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Autophagosome\_0} = v_{46} + v_{47} + v_{48} + v_{49} - v_{37} \tag{317}$$

9.75 Species Proteasome_0

Name Proteasome

Notes Proteasome

Initial concentration 1.5 dimensionless · dimensionless^{-1}

This species takes part in 20 reactions (as a modifier in J4, J4, J4, J4, J4, J4, J4, J4, J4, J4, J38, J38, J38, J38, J38, J38, J38, J38, J38, J38), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Proteasome\_0} = 0 \tag{318}$$

9.76 Species Lysosome_0

Name Lysosome

Notes Lysosome

Initial concentration 2.5 dimensionless · dimensionless^{-1}

This species takes part in 40 reactions (as a modifier in J36, J36, J36, J36, J36, J36, J36, J36, J36, J36, J46, J46, J46, J46, J46, J46, J46, J46, J46, J46, J47, J47, J47, J47, J47, J47, J47, J47, J47, J47, J48, J48, J48, J48, J48, J48, J48, J48, J48, J48), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Lysosome\_0} = 0 \tag{319}$$

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