SBML Model Report

Model name: “Proctor2005 - Actions of chaperones and their role in ageing”

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Carole Proctor[1] and Enuo He[2] at February 26th 2007 at 1:30 p. m. and last time modified at June third 2014 at 8:38 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	1
species types	0	species	16
events	0	constraints	0
reactions	23	function definitions	0
global parameters	21	unit definitions	1
rules	0	initial assignments	0

Model Notes

Proctor2005 - Actions of chaperones and theirrole in ageing

This model is described in the article:Modelling the actions of chaperones and their role in ageing.Proctor CJ, Soti C, Boys RJ, Gillespie CS, Shanley DP, Wilkinson DJ, Kirkwood TB.Mech. Ageing Dev. 2005 Jan; 126(1): 119-131

[1]University of Newcastle, c.j.proctor@ncl.ac.uk
[2]BNMC, enuo@caltech.edu

Abstract:

Many molecular chaperones are also known as heat shock proteins because they are synthesised in increased amounts after brief exposure of cells to elevated temperatures. They have many cellular functions and are involved in the folding of nascent proteins, the re-folding of denatured proteins, the prevention of protein aggregation, and assisting the targeting of proteins for degradation by the proteasome and lysosomes. They also have a role in apoptosis and are involved in modulating signals for immune and inflammatory responses. Stress-induced transcription of heat shock proteins requires the activation of heat shock factor (HSF). Under normal conditions, HSF is bound to heat shock proteins resulting in feedback repression. During stress, cellular proteins undergo denaturation and sequester heat shock proteins bound to HSF, which is then able to become transcriptionally active. The induction of heat shock proteins is impaired with age and there is also a decline in chaperone function. Aberrant/damaged proteins accumulate with age and are implicated in several important age-related conditions (e.g. Alzheimer's disease, Parkinson's disease, and cataract). Therefore, the balance between damaged proteins and available free chaperones may be greatly disturbed during ageing. We have developed a mathematical model to describe the heat shock system. The aim of the model is two-fold: to explore the heat shock system and its implications in ageing; and to demonstrate how to build a model of a biological system using our simulation system (biology of ageing e-science integration and simulation (BASIS)).

This model is hosted on BioModels Database and identified by: BIOMD0000000091.

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

2.1 Unit `substance`

Definition item

2.2 Unit `volume`

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

Definition l

2.3 Unit `area`

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

Definition m^2

2.4 Unit `length`

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

Definition m

2.5 Unit `time`

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

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`compartment`			3	1	litre	☑	

3.1 Compartment `compartment`

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

4 Species

This model contains 16 species. The boundary condition of one of these species is set to `true` so that this species' amount cannot be changed by any reaction. Section 7 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
`Hsp90`	Hsp90	`compartment`	item	⊟	⊟
`HCom`	HCom	`compartment`	item	⊟	⊟
`HSF1`	HSF1	`compartment`	item	⊟	⊟
`MisP`	MisP	`compartment`	item	⊟	⊟
`MCom`	MCom	`compartment`	item	⊟	⊟
`TriH`	TriH	`compartment`	item	⊟	⊟
`DiH`	DiH	`compartment`	item	⊟	⊟
`NatP`	NatP	`compartment`	item	⊟	⊟
`AggP`	AggP	`compartment`	item	⊟	⊟
`HSE`	HSE	`compartment`	item	⊟	⊟
`HSETriH`	HSETriH	`compartment`	item	⊟	⊟
`X`	X	`compartment`	item	⊟	⊟
`ROS`	ROS	`compartment`	item	⊟	⊟
`ATP`	ATP	`compartment`	item	⊟	⊟
`ADP`	ADP	`compartment`	item	⊟	⊟
`source`	source	`compartment`	item	⊟	☑

5 Parameters

This model contains 21 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		10.000		☑
k2	k2		$2 \cdot 10^{-5}$		☑
k3	k3		50.000		☑
k4	k4		10^{-5}		☑
k5	k5		$4 \cdot 10^{-6}$		☑
k6	k6		$6 \cdot 10^{-7}$		☑
k7	k7		10^{-7}		☑
k8	k8		500.000		☑
k9	k9		1.000		☑
k10	k10		0.010		☑
k11	k11		100.000		☑
k12	k12		0.500		☑
k13	k13		0.500		☑
k14	k14		0.050		☑
k15	k15		0.080		☑
k16	k16		1000.000		☑
k17	k17		$8.02 \cdot 10^{-9}$		☑
k18	k18		12.000		☑
k19	k19		0.020		☑
k20	k20		0.100		☑
k21	k21		0.001		☑

6 Reactions

This model contains 23 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	proteinSynthesis	proteinSynthesis	0 source $\longrightarrow$ NatP	
2	misfolding	misfolding	NatP + ROS $\longrightarrow$ MisP + ROS	
3	Hsp90MisPBinding	Hsp90MisPBinding	MisP + Hsp90 $\longrightarrow$ MCom	
4	unsuccessulRefolding	unsuccessfulRefolding	MCom $\longrightarrow$ MisP + Hsp90	
5	refolding	refolding	MCom + ATP $\longrightarrow$ Hsp90 + NatP + ADP	
6	proteinDegradation	proteinDegradation	MisP + ATP $\longrightarrow$ ADP	
7	proteinAggregation1		2 MisP $\longrightarrow$ AggP	
8	proteinAggregation2		MisP + AggP $\longrightarrow$ 2 AggP	
9	Hsp90HSF1Binding	Hsp90HSF1Binding	Hsp90 + HSF1 $\longrightarrow$ HCom	
10	Hsp90HSF1Release	Hsp90HSF1Release	HCom $\longrightarrow$ Hsp90 + HSF1	
11	dimerisation	dimerisation	2 HSF1 $\longrightarrow$ DiH	
12	trimerisation	trimerisation	HSF1 + DiH $\longrightarrow$ TriH	
13	deTrimerisation	deTrimerisation	TriH $\longrightarrow$ HSF1 + DiH	
14	deDimerisation	deDimerisation	DiH $\longrightarrow$ 2 HSF1	
15	HSETriHBinding	HSETriHBinding	TriH + HSE $\longrightarrow$ HSETriH	
16	HSETriHRelease	HSETriHRelease	HSETriH $\longrightarrow$ HSE + TriH	
17	Hsp90Transcription	Hsp90Transcription	HSETriH $\longrightarrow$ HSETriH + Hsp90	
18	Hsp90Degradation	Hsp90Degradation	Hsp90 + ATP $\longrightarrow$ ADP	
19	countTime	countTime	0 source $\longrightarrow$ X	
20	ATPformation	ATPformation	ADP $\longrightarrow$ ATP	
21	ATPconsumption	ATPconsumption	ATP $\longrightarrow$ ADP	
22	radicalFormation	radicalFormation	0 source $\longrightarrow$ ROS	
23	radicalScavenging	radicalScavenging	ROS $\longrightarrow \emptyset$	

№	Id	Name	Reaction Equation	SBO

6.1 Reaction `proteinSynthesis`

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

Name proteinSynthesis

Reaction equation

$$0\,\text{source} \longrightarrow \text{NatP} \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
`source`	source	

Product

Table 7: Properties of each product.

Id	Name	SBO
`NatP`	NatP	

Kinetic Law

Derived unit not available

$$v_1 = \text{k1} \tag{2}$$

6.2 Reaction `misfolding`

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

Name misfolding

Reaction equation

$$\text{NatP} + \text{ROS} \longrightarrow \text{MisP} + \text{ROS} \tag{3}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
NatP	NatP	
ROS	ROS	

Products

Table 9: Properties of each product.

Id	Name	SBO
MisP	MisP	
ROS	ROS	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{k2} \cdot \mathrm{NatP} \cdot \mathrm{ROS} \tag{4}$$

6.3 Reaction Hsp90MisPBinding

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

Name Hsp90MisPBinding

Reaction equation

$$\mathrm{MisP} + \mathrm{Hsp90} \longrightarrow \mathrm{MCom} \tag{5}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
MisP	MisP	
Hsp90	Hsp90	

Product

Table 11: Properties of each product.

Id	Name	SBO
MCom	MCom	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{k3} \cdot \mathrm{MisP} \cdot \mathrm{Hsp90} \tag{6}$$

6.4 Reaction unsuccessulRefolding

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

Name unsuccessfulRefolding

Reaction equation

$$\mathrm{MCom} \longrightarrow \mathrm{MisP} + \mathrm{Hsp90} \tag{7}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
MCom	MCom	

Products

Table 13: Properties of each product.

Id	Name	SBO
MisP	MisP	
Hsp90	Hsp90	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{k4} \cdot \mathrm{MCom} \tag{8}$$

6.5 Reaction refolding

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

Name refolding

Reaction equation

$$\mathrm{MCom} + \mathrm{ATP} \longrightarrow \mathrm{Hsp90} + \mathrm{NatP} + \mathrm{ADP} \tag{9}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
MCom	MCom	
ATP	ATP	

Products

Table 15: Properties of each product.

Id	Name	SBO
Hsp90	Hsp90	
NatP	NatP	
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{k5} \cdot \mathrm{MCom} \cdot \mathrm{ATP} \tag{10}$$

6.6 Reaction proteinDegradation

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

Name proteinDegradation

Reaction equation

$$\mathrm{MisP} + \mathrm{ATP} \longrightarrow \mathrm{ADP} \tag{11}$$

Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
MisP	MisP	
ATP	ATP	

Product

Table 17: Properties of each product.

Id	Name	SBO
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{k6} \cdot \mathrm{MisP} \cdot \mathrm{ATP} \tag{12}$$

6.7 Reaction proteinAggregation1

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

Reaction equation

$$2\,\mathrm{MisP} \longrightarrow \mathrm{AggP} \tag{13}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
MisP	MisP	

Product

Table 19: Properties of each product.

Id	Name	SBO
AggP	AggP	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{(\mathrm{MisP} - 1) \cdot \mathrm{k7} \cdot \mathrm{MisP}}{2} \tag{14}$$

6.8 Reaction `proteinAggregation2`

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

Reaction equation

$$\mathrm{MisP} + \mathrm{AggP} \longrightarrow 2\,\mathrm{AggP} \tag{15}$$

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
`MisP`	MisP	
`AggP`	AggP	

Product

Table 21: Properties of each product.

Id	Name	SBO
`AggP`	AggP	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{k7} \cdot \mathrm{MisP} \cdot \mathrm{AggP} \tag{16}$$

6.9 Reaction `Hsp90HSF1Binding`

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

Name Hsp90HSF1Binding

Reaction equation

$$\mathrm{Hsp90} + \mathrm{HSF1} \longrightarrow \mathrm{HCom} \tag{17}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
Hsp90	Hsp90	
HSF1	HSF1	

Product

Table 23: Properties of each product.

Id	Name	SBO
HCom	HCom	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{k8} \cdot \mathrm{Hsp90} \cdot \mathrm{HSF1} \tag{18}$$

6.10 Reaction Hsp90HSF1Release

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

Name Hsp90HSF1Release

Reaction equation

$$\mathrm{HCom} \longrightarrow \mathrm{Hsp90} + \mathrm{HSF1} \tag{19}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
HCom	HCom	

Products

Table 25: Properties of each product.

Id	Name	SBO
Hsp90	Hsp90	
HSF1	HSF1	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{k9} \cdot \mathrm{HCom} \tag{20}$$

6.11 Reaction dimerisation

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

Name dimerisation

Reaction equation

$$2\,\mathrm{HSF1} \longrightarrow \mathrm{DiH} \tag{21}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
HSF1	HSF1	

Product

Table 27: Properties of each product.

Id	Name	SBO
DiH	DiH	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \frac{(\mathrm{HSF1} - 1) \cdot \mathrm{k10} \cdot \mathrm{HSF1}}{2} \tag{22}$$

6.12 Reaction `trimerisation`

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

Name trimerisation

Reaction equation

$$\mathrm{HSF1} + \mathrm{DiH} \longrightarrow \mathrm{TriH} \tag{23}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
`HSF1`	HSF1	
`DiH`	DiH	

Product

Table 29: Properties of each product.

Id	Name	SBO
`TriH`	TriH	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{k11} \cdot \mathrm{HSF1} \cdot \mathrm{DiH} \tag{24}$$

6.13 Reaction `deTrimerisation`

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

Name deTrimerisation

Reaction equation

$$\mathrm{TriH} \longrightarrow \mathrm{HSF1} + \mathrm{DiH} \tag{25}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
TriH	TriH	

Products

Table 31: Properties of each product.

Id	Name	SBO
HSF1	HSF1	
DiH	DiH	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{k12} \cdot \mathrm{TriH} \tag{26}$$

6.14 Reaction deDimerisation

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

Name deDimerisation

Reaction equation

$$\mathrm{DiH} \longrightarrow 2\,\mathrm{HSF1} \tag{27}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
DiH	DiH	

Product

Table 33: Properties of each product.

Id	Name	SBO
HSF1	HSF1	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{k13} \cdot \mathrm{DiH} \tag{28}$$

6.15 Reaction HSETriHBinding

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

Name HSETriHBinding

Reaction equation

$$\mathrm{TriH} + \mathrm{HSE} \longrightarrow \mathrm{HSETriH} \tag{29}$$

Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
TriH	TriH	
HSE	HSE	

Product

Table 35: Properties of each product.

Id	Name	SBO
HSETriH	HSETriH	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{k14} \cdot \mathrm{HSE} \cdot \mathrm{TriH} \tag{30}$$

6.16 Reaction HSETriHRelease

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

Name HSETriHRelease

Reaction equation

$$\mathrm{HSETriH} \longrightarrow \mathrm{HSE} + \mathrm{TriH} \tag{31}$$

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
HSETriH	HSETriH	

Products

Table 37: Properties of each product.

Id	Name	SBO
HSE	HSE	
TriH	TriH	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{k15} \cdot \mathrm{HSETriH} \tag{32}$$

6.17 Reaction Hsp90Transcription

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

Name Hsp90Transcription

Reaction equation

$$\mathrm{HSETriH} \longrightarrow \mathrm{HSETriH} + \mathrm{Hsp90} \tag{33}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
HSETriH	HSETriH	

Products

Table 39: Properties of each product.

Id	Name	SBO
HSETriH	HSETriH	
Hsp90	Hsp90	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{k16} \cdot \mathrm{HSETriH} \tag{34}$$

6.18 Reaction Hsp90Degradation

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

Name Hsp90Degradation

Reaction equation

$$\mathrm{Hsp90} + \mathrm{ATP} \longrightarrow \mathrm{ADP} \tag{35}$$

Reactants

Table 40: Properties of each reactant.

Id	Name	SBO
Hsp90	Hsp90	
ATP	ATP	

Product

Table 41: Properties of each product.

Id	Name	SBO
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{k17} \cdot \mathrm{Hsp90} \cdot \mathrm{ATP} \tag{36}$$

6.19 Reaction `countTime`

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

Name countTime

Reaction equation

$$0\,\mathrm{source} \longrightarrow \mathrm{X} \tag{37}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
`source`	source	

Product

Table 43: Properties of each product.

Id	Name	SBO
`X`	X	

Kinetic Law

Derived unit not available

$$v_{19} = 1 \tag{38}$$

6.20 Reaction `ATPformation`

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

Name ATPformation

Reaction equation

$$\mathrm{ADP} \longrightarrow \mathrm{ATP} \tag{39}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
ADP	ADP	

Product

Table 45: Properties of each product.

Id	Name	SBO
ATP	ATP	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \mathrm{k18} \cdot \mathrm{ADP} \tag{40}$$

6.21 Reaction ATPconsumption

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

Name ATPconsumption

Reaction equation

$$\mathrm{ATP} \longrightarrow \mathrm{ADP} \tag{41}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
ATP	ATP	

Product

Table 47: Properties of each product.

Id	Name	SBO
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{k19} \cdot \mathrm{ATP} \tag{42}$$

6.22 Reaction `radicalFormation`

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

Name radicalFormation

Reaction equation

$$0\,\mathrm{source} \longrightarrow \mathrm{ROS} \tag{43}$$

Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
`source`	source	

Product

Table 49: Properties of each product.

Id	Name	SBO
`ROS`	ROS	

Kinetic Law

Derived unit not available

$$v_{22} = \mathrm{k20} \tag{44}$$

6.23 Reaction `radicalScavenging`

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

Name radicalScavenging

Reaction equation

$$\mathrm{ROS} \longrightarrow \emptyset \tag{45}$$

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
ROS	ROS	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{k21} \cdot \text{ROS} \tag{46}$$

7 Derived Rate Equations

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

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

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

7.1 Species Hsp90

Name Hsp90

Initial amount 300000 item

This species takes part in seven reactions (as a reactant in Hsp90MisPBinding, Hsp90HSF1Binding, Hsp90Degradation and as a product in unsuccessulRefolding, refolding, Hsp90HSF1Release, Hsp90Transcription).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Hsp90} = v_4 + v_5 + v_{10} + v_{17} - v_3 - v_9 - v_{18} \tag{47}$$

7.2 Species HCom

Name HCom

Initial amount 5900 item

This species takes part in two reactions (as a reactant in Hsp90HSF1Release and as a product in Hsp90HSF1Binding).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{HCom} = v_9 - v_{10} \tag{48}$$

7.3 Species HSF1

Name HSF1

Initial amount 100 item

This species takes part in six reactions (as a reactant in Hsp90HSF1Binding, dimerisation, trimerisation and as a product in Hsp90HSF1Release, deTrimerisation, deDimerisation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{HSF1} = v_{10} + v_{13} + 2\,v_{14} - v_9 - 2\,v_{11} - v_{12} \tag{49}$$

7.4 Species MisP

Name MisP

Initial amount 0 item

This species takes part in six reactions (as a reactant in Hsp90MisPBinding, proteinDegradation, proteinAggregation1, proteinAggregation2 and as a product in misfolding, unsuccessulRefolding).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MisP} = v_2 + v_4 - v_3 - v_6 - 2\,v_7 - v_8 \tag{50}$$

7.5 Species MCom

Name MCom

Initial amount 0 item

This species takes part in three reactions (as a reactant in unsuccessulRefolding, refolding and as a product in Hsp90MisPBinding).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MCom} = v_3 - v_4 - v_5 \tag{51}$$

7.6 Species TriH

Name TriH

Initial amount 0 item

This species takes part in four reactions (as a reactant in deTrimerisation, HSETriHBinding and as a product in trimerisation, HSETriHRelease).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TriH} = v_{12} + v_{16} - v_{13} - v_{15} \tag{52}$$

7.7 Species DiH

Name DiH

Initial amount 0 item

This species takes part in four reactions (as a reactant in trimerisation, deDimerisation and as a product in dimerisation, deTrimerisation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DiH} = v_{11} + v_{13} - v_{12} - v_{14} \tag{53}$$

7.8 Species NatP

Name NatP

Initial amount 6000000 item

This species takes part in three reactions (as a reactant in misfolding and as a product in proteinSynthesis, refolding).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NatP} = v_{1} + v_{5} - v_{2} \tag{54}$$

7.9 Species AggP

Name AggP

Initial amount 0 item

This species takes part in three reactions (as a reactant in proteinAggregation2 and as a product in proteinAggregation1, proteinAggregation2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AggP} = v_{7} + 2\,v_{8} - v_{8} \tag{55}$$

7.10 Species HSE

Name HSE

Initial amount 1 item

This species takes part in two reactions (as a reactant in HSETriHBinding and as a product in HSETriHRelease).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{HSE} = v_{16} - v_{15} \tag{56}$$

7.11 Species HSETriH

Name HSETriH

Initial amount 0 item

This species takes part in four reactions (as a reactant in HSETriHRelease, Hsp90Transcription and as a product in HSETriHBinding, Hsp90Transcription).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{HSETriH} = v_{15} + v_{17} - v_{16} - v_{17} \tag{57}$$

7.12 Species X

Name X

Initial amount 0 item

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = v_{19} \tag{58}$$

7.13 Species ROS

Name ROS

Initial amount 100 item

This species takes part in four reactions (as a reactant in misfolding, radicalScavenging and as a product in misfolding, radicalFormation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ROS} = v_{2} + v_{22} - v_{2} - v_{23} \tag{59}$$

7.14 Species ATP

Name ATP

Initial amount 10000 item

This species takes part in five reactions (as a reactant in refolding, proteinDegradation, Hsp90Degradation, ATPconsumption and as a product in ATPformation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = v_{20} - v_{5} - v_{6} - v_{18} - v_{21} \tag{60}$$

7.15 Species ADP

Name ADP

Initial amount 1000 item

This species takes part in five reactions (as a reactant in ATPformation and as a product in refolding, proteinDegradation, Hsp90Degradation, ATPconsumption).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = v_5 + v_6 + v_{18} + v_{21} - v_{20} \tag{61}$$

7.16 Species source

Name source

Initial amount 0 item

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{source} = 0 \tag{62}$$

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

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany