define@key

SBML Model Report

Model name: "Crespo2012 - Kinetics of Amyloid Fibril Formation"

September 9, 2014

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 July 17th 2014 at 5:11 p. m. and last time modified at September eighth 2014 at 2:06 p. m. Table 1 shows an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	1
events	0	constraints	0
reactions	0	function definitions	0
global parameters	4	unit definitions	3
rules	3	initial assignments	0

Model Notes

Crespo2012 - Kinetics of Amyloid FibrilFormation

This model is described in the article:A generic crystallization-like model that describes the kinetics of amyloid fibril formation.Crespo R, Rocha FA, Damas AM, Martins PM.J. Biol. Chem. 2012 Aug; 287(36): 30585-30594

Abstract:

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Associated with neurodegenerative disorders such as Alzheimer, Parkinson, or prion diseases, the conversion of soluble proteins into amyloid fibrils remains poorly understood. Extensive „in vitro„ measurements of protein aggregation kinetics have been reported, but no consensus mechanism has emerged until now. This contribution aims at overcoming this gap by proposing a theoretically consistent crystallization-like model (CLM) that is able to describe the classic types of amyloid fibrillization kinetics identified in our literature survey. Amyloid conversion represented as a function of time is shown to follow different curve shapes, ranging from sigmoidal to hyperbolic, according to the relative importance of the nucleation and growth steps. Using the CLM, apparently unrelated data are deconvoluted into generic mechanistic information integrating the combined influence of seeding, nucleation, growth, and fibril breakage events. It is notable that this complex assembly of interdependent events is ultimately reduced to a mathematically simple model, whose two parameters can be determined by little more than visual inspection. The good fitting results obtained for all cases confirm the CLM as a good approximation to the generalized underlying principle governing amyloid fibrillization. A perspective is presented on possible applications of the CLM during the development of new targets for amyloid disease therapeutics.

This model is hosted on BioModels Database and identified by: BIOMD0000000531.

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 ml

2.2 Unit `time`

Name time

Definition 3600 s

2.3 Unit `substance`

Name substance

Definition mmol

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 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

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

3.1 Compartment `Cell`

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

Name Cell

4 Species

This model contains one 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
`alpha`	alpha	`Cell`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	☑

5 Parameters

This model contains four global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Ka`	Ka		1.440		☑
`kb`	kb		$1.6 \cdot 10^{-10}$		☑
`kat50`	kat50		22.556		☐
`v50t50`	v50t50		5.639		☐

6 Rules

This is an overview of three rules.

6.1 Rule `kat50`

Rule `kat50` is an assignment rule for parameter `kat50`:

$$\text{kat50} = \left(\frac{1}{\text{kb}} + 1\right) \tag{1}$$

Derived unit dimensionless

6.2 Rule `v50t50`

Rule `v50t50` is an assignment rule for parameter `v50t50`:

$$\text{v50t50} = \frac{1}{4} \cdot (\text{kb} + 1) \cdot \left(\frac{1}{\text{kb}} + 1\right) \tag{2}$$

6.3 Rule `alpha`

Rule `alpha` is an assignment rule for species `alpha`:

$$\text{alpha} = 1 - \frac{1}{\text{kb} \cdot (\exp(\text{Ka} \cdot \text{time}) - 1) + 1} \tag{3}$$

7 Derived Rate Equation

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

7.1 Species alpha

Name alpha

Initial concentration $0\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

Involved in rule alpha

One rule determines the species' quantity.

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.

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