**SBML Model Report**

# Model name: “Auer2010 - Correlation between lag time and aggregation rate in protein aggregation”

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 November tenth 2014 at 2:26 p. m. and last time modified at April eighth 2016 at 5:42 p. m. Table 1 provides 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 | 8 | unit definitions | 3 |
| rules | 4 | initial assignments | 0 |

### Model Notes

Auer2010 - Correlation between lag time andaggregation rate in protein aggregation

This model is described in the article:Insight into the correlation between lag time and aggregation rate in the kinetics of protein aggregation.Auer S, Kashchiev D.Proteins 2010 Aug; 78(11): 2412-2416

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Abstract:

Under favorable conditions, many proteins can assemble into macroscopically large aggregates such as the amyloid fibrils that are associated with Alzheimer's, Parkinson's, and other neurological and systemic diseases. The overall process of protein aggregation is characterized by initial lag time during which no detectable aggregation occurs in the solution and by maximal aggregation rate at which the dissolved protein converts into aggregates. In this study, the correlation between the lag time and the maximal rate of protein aggregation is analyzed. It is found that the product of these two quantities depends on a single numerical parameter, the kinetic index of the curve quantifying the time evolution of the fraction of protein aggregated. As this index depends relatively little on the conditions and/or system studied, our finding provides insight into why for many experiments the values of the product of the lag time and the maximal aggregation rate are often equal or quite close to each other. It is shown how the kinetic index is related to a basic kinetic parameter of a recently proposed theory of protein aggregation.



## 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 |
|---|---|---|---|---|---|---|---|
| `Brain` | Brain | | 3 | 1 | litre | ☑ | |

### 3.1 Compartment `Brain`

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

**Name** Brain

## 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 |
|---|---|---|---|---|---|
| `Amyloid` | Amyloid | `Brain` | $\mathrm{mmol} \cdot \mathrm{ml}^{-1}$ | ⊟ | ☑ |

# 5 Parameters

This model contains eight global parameters.

Table 4: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| omega | omega | | 35.300 | | ☑ |
| n | n | | 7.200 | | ☑ |
| a | a | | 2.043 | | ☐ |
| e | e | | 2.718 | | ☑ |
| k | k | | 0.205 | | ☑ |
| ka | ka | | 0.075 | | ☐ |
| C | C+ | | $6.9 \cdot 10^{-4}$ | | ☑ |
| t1 | t1 | | 27.126 | | ☐ |

# 6 Rules

This is an overview of four rules.

## 6.1 Rule Amyloid

Rule Amyloid is an assignment rule for species Amyloid:

$$\text{Amyloid} = 1 - \exp\left(\left(\left(\frac{\text{time}}{\text{omega}}\right)^{\text{n}}\right)\right) \tag{1}$$

## 6.2 Rule a

Rule a is an assignment rule for parameter a:

$$\text{a} = \text{n} \cdot \exp\left(\frac{(\text{n}-1)}{\text{n}}\right) - 1 \tag{2}$$

## 6.3 Rule ka

Rule ka is an assignment rule for parameter ka:

$$\text{ka} = \frac{\text{k}}{\text{e}} \tag{3}$$

## 6.4 Rule t1

Rule t1 is an assignment rule for parameter t1:

$$\text{t1} = \left(\left(\frac{1}{\text{C}}\right) - \text{e} + 1\right) \cdot \frac{1}{\text{k}} \tag{4}$$

# 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 `Amyloid`

**Name** Amyloid

**Notes** `Amyloid fibrils or other aggregates`

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

**Involved in rule** `Amyloid`

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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