SBML Model Report

Model name: “Kamihira2000”

August 15, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Thawfeek Varusai[1] at August eighth 2016 at 3:40 p. m. and last time modified at August 15th 2016 at 11:38 a. m. Table 1 shows an overview of the quantities of all components of this model.

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

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

Model Notes

Kamihira2000 - calcitonin fibrillation kinetics

This model studies the kinetics of human calcitonin fibrillation described as a two-step process. Empirical data is used to determine the parameter values. Results show that the first step in fibrillation is a slow homogenous reaction and the second step is a fast autocatalytic heterogenous reaction.

This model is described in the article:Conformational transitions and fibrillation mechanism of human calcitonin as studied by high-resolution solid-state 13C NMR.Kamihira M, Naito A, Tuzi S, Nosaka AY, Sait H.Protein Sci. 2000 May; 9(5): 867-877

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Abstract:

Conformational transitions of human calcitonin (hCT) during fibril formation in the acidic and neutral conditions were investigated by high-resolution solid-state 13C NMR spectroscopy. In aqueous acetic acid solution (pH 3.3), a local alpha-helical form is present around Gly10 whereas a random coil form is dominant as viewed from Phe22, Ala26, and Ala31 in the monomer form on the basis of the 13C chemical shifts. On the other hand, a local beta-sheet form as viewed from Gly10 and Phe22, and both beta-sheet and random coil as viewed from Ala26 and Ala31 were detected in the fibril at pH 3.3. The results indicate that conformational transitions from alpha-helix to beta-sheet, and from random coil to beta-sheet forms occurred in the central and C-terminus regions, respectively, during the fibril formation. The increased 13C resonance intensities of fibrils after a certain delay time suggests that the fibrillation can be explained by a two-step reaction mechanism in which the first step is a homogeneous association to form a nucleus, and the second step is an autocatalytic heterogeneous fibrillation. In contrast to the fibril at pH 3.3, the fibril at pH 7.5 formed a local beta-sheet conformation at the central region and exhibited a random coil at the C-terminus region. Not only a hydrophobic interaction among the amphiphilic alpha-helices, but also an electrostatic interaction between charged side chains can play an important role for the fibril formation at pH 7.5 and 3.3 acting as electrostatically favorable and unfavorable interactions, respectively. These results suggest that hCT fibrils are formed by stacking antiparallel beta-sheets at pH 7.5 and a mixture of antiparallel and parallel beta-sheets at pH 3.3.

2 Unit Definitions

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

2.1 Unit `substance`

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

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_	compartment_		3	1	litre	☑	

3.1 Compartment compartment_

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

Name compartment_

4 Species

This model contains one species. Section 8 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
f	fibril fraction	compartment_	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains three global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$2.79 \cdot 10^{-6}$		☑
k2	k2		2.290		☑
a	a		$5.85 \cdot 10^{-5}$		☑

6 Function definitions

This is an overview of four function definitions.

6.1 Function definition Constant_flux__reversible

Name Constant flux (reversible)

Argument v

Mathematical Expression

$$\mathrm{v} \tag{1}$$

6.2 Function definition Function_for_R2

Name Function for R2

Arguments a, [f], k2

Mathematical Expression

$$\mathrm{k2} \cdot \mathrm{a} \cdot [\mathrm{f}] \tag{2}$$

6.3 Function definition Function_for_R3

Name Function for R3

Arguments [f], k1

Mathematical Expression

$$\mathrm{k1} \cdot [\mathrm{f}] \tag{3}$$

6.4 Function definition Function_for_R4

Name Function for R4

Arguments a, [f], k2

Mathematical Expression

$$k2 \cdot a \cdot [f] \cdot [f] \tag{4}$$

7 Reactions

This model contains four 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	R1	R1	$\emptyset \rightleftharpoons f$	
2	R2	R2	$\emptyset \rightleftharpoons f$	
3	R3	R3	$f \rightleftharpoons \emptyset$	
4	R4	R4	$f \rightleftharpoons \emptyset$	

7.1 Reaction R1

This is a reversible reaction of no reactant forming one product.

Name R1

Reaction equation

$$\emptyset \rightleftharpoons \mathrm{f} \tag{5}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
f	fibril fraction	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\left(\mathrm{compartment\_}\right) \cdot \mathrm{Constant\_flux\_\_reversible}\left(\mathrm{k1}\right) \tag{6}$$

$$\mathrm{Constant\_flux\_\_reversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{7}$$

$$\mathrm{Constant\_flux\_\_reversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{8}$$

7.2 Reaction R2

This is a reversible reaction of no reactant forming one product.

Name R2

Reaction equation

$$\emptyset \rightleftharpoons \mathrm{f} \tag{9}$$

Product

Table 7: Properties of each product.

Id	Name	SBO
f	fibril fraction	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{compartment\_}) \cdot \mathrm{Function\_for\_R2}\,(\mathrm{a}, [\mathrm{f}], \mathrm{k2}) \tag{10}$$

$$\mathrm{Function\_for\_R2}\,(\mathrm{a}, [\mathrm{f}], \mathrm{k2}) = \mathrm{k2} \cdot \mathrm{a} \cdot [\mathrm{f}] \tag{11}$$

$$\mathrm{Function\_for\_R2}\,(\mathrm{a}, [\mathrm{f}], \mathrm{k2}) = \mathrm{k2} \cdot \mathrm{a} \cdot [\mathrm{f}] \tag{12}$$

7.3 Reaction R3

This is a reversible reaction of one reactant forming no product.

Name R3

Reaction equation

$$\mathrm{f} \rightleftharpoons \emptyset \tag{13}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
f	fibril fraction	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment\_}) \cdot \mathrm{Function\_for\_R3}\,([\mathrm{f}], \mathrm{k1}) \tag{14}$$

$$\mathrm{Function\_for\_R3}\,([\mathrm{f}], \mathrm{k1}) = \mathrm{k1} \cdot [\mathrm{f}] \tag{15}$$

$$\mathrm{Function\_for\_R3}\,([\mathrm{f}], \mathrm{k1}) = \mathrm{k1} \cdot [\mathrm{f}] \tag{16}$$

7.4 Reaction R4

This is a reversible reaction of one reactant forming no product.

Name R4

Reaction equation

$$\mathrm{f} \rightleftharpoons \emptyset \tag{17}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
f	fibril fraction	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\left(\mathrm{compartment\_}\right) \cdot \mathrm{Function\_for\_R4}\left(\mathrm{a}, [\mathrm{f}], \mathrm{k2}\right) \tag{18}$$

$$\mathrm{Function\_for\_R4}\left(\mathrm{a}, [\mathrm{f}], \mathrm{k2}\right) = \mathrm{k2} \cdot \mathrm{a} \cdot [\mathrm{f}] \cdot [\mathrm{f}] \tag{19}$$

$$\mathrm{Function\_for\_R4}\left(\mathrm{a}, [\mathrm{f}], \mathrm{k2}\right) = \mathrm{k2} \cdot \mathrm{a} \cdot [\mathrm{f}] \cdot [\mathrm{f}] \tag{20}$$

8 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.

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.

8.1 Species `f`

Name fibril fraction

Notes `This species indicates the fraction of human calcitonin in the system.`

Initial concentration $0\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in R3, R4 and as a product in R1, R2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{f} = v_1 + v_2 - v_3 - v_4 \tag{21}$$

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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