SBML Model Report

Model name: "Brown1997 - Plasma Melatonin Levels"

May 17, 2018

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Matthew Grant Roberts[1] and Catherine Lloyd[2] at June 25th 2010 at 12:29 a. m. and last time modified at June 25th 2010 at 12:29 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	0
events	0	constraints	0
reactions	0	function definitions	0
global parameters	14	unit definitions	1
rules	7	initial assignments	0

Model Notes

Brown1997 - Plasma Melatonin LevelsA mathematical model that incorporatesa piecewise function for NAT activity to predict melatoninconcentration.

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This model is described in the article:A mathematical model of diurnal variations in human plasma melatonin levels.Brown EN, Choe Y, Shanahan TL, Czeisler CA.Am. J. Physiol. 1997 Mar; 272(3 Pt 1): E506-16

Abstract:

Studies in animals and humans suggest that the diurnal pattern in plasma melatonin levels is due to the hormone's rates of synthesis, circulatory infusion and clearance, circadian control of synthesis onset and offset, environmental lighting conditions, and error in the melatonin immunoassay. A two-dimensional linear differential equation model of the hormone is formulated and is used to analyze plasma melatonin levels in 18 normal healthy male subjects during a constant routine. Recently developed Bayesian statistical procedures are used to incorporate correctly the magnitude of the immunoassay error into the analysis. The estimated parameters [median (range)] were clearance half-life of 23.67 (14.79-59.93) min, synthesis onset time of 2206 (1940-0029), synthesis offset time of 0621 (0246-0817), and maximum N-acetyltransferase activity of 7.17(2.34-17.93) pmol x l(-1) x min(-1). All were in good agreement with values from previous reports. The difference between synthesis offset time and the phase of the core temperature minimum was 1 h 15 min (-4 h 38 min-2 h 43 min). The correlation between synthesis onset and the dim light melatonin onset was 0.93. Our model provides a more physiologically plausible estimate of the melatonin synthesis onset time than that given by the dim light melatonin onset and the first reliable means of estimating the phase of synthesis offset. Our analysis shows that the circadian and pharmacokinetics parameters of melatonin can be reliably estimated from a single model.

This model is hosted on BioModels Database and identified by: BIOMD0000000672.

To cite BioModels Database, please use: Chelliah V et al. BioModels: ten-year anniversary. Nucl. Acids Res. 2015, 43(Database issue):D542-8.

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 `time`

Name time

Definition 60 s

2.2 Unit `substance`

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

Definition mol

2.3 Unit `volume`

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

Definition l

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
`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 Parameters

This model contains 14 global parameters.

Table 3: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`H1`	H1		0.050		☐
`H2`	H2		1.000		☐

Id	Name	SBO	Value	Unit	Constant
`A`	A		0.000		☐
`t_on`	t_on		1316.000		☑
`t_off`	t_off		1794.000		☑
`A_max`	A_max		6.510		☑
`beta_I`	beta_I		0.246		☐
`beta_C`	beta_C		0.029		☐
`alpha`	alpha		0.027		☐
`lamda`	lamda		0.029		☐
`tau_I`	tau_I		2.820		☑
`tau_C`	tau_C		23.670		☑
`tau_alpha`	tau_alpha		25.920		☑
`tau_lamda`	tau_lamda		24.040		☑

5 Rules

This is an overview of seven rules.

5.1 Rule `beta_I`

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

$$\text{beta\_I} = \frac{\ln 2}{\text{tau\_I}} \tag{1}$$

5.2 Rule `beta_C`

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

$$\text{beta\_C} = \frac{\ln 2}{\text{tau\_C}} \tag{2}$$

5.3 Rule `alpha`

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

$$\text{alpha} = \frac{\ln 2}{\text{tau\_alpha}} \tag{3}$$

5.4 Rule `lamda`

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

$$\text{lamda} = \frac{\ln 2}{\text{tau\_lamda}} \tag{4}$$

5.5 Rule A

Rule A is an assignment rule for parameter A:

$$A = \begin{cases} \mathrm{A\_max} \cdot \dfrac{1 - \exp\left(\mathrm{lamda} \cdot \left(\mathrm{time} - \mathrm{t\_on}\right)\right)}{1 - \exp\left(\mathrm{lamda} \cdot \left(\mathrm{t\_off} - \mathrm{t\_on}\right)\right)} & \text{if } \left(\mathrm{time} < \mathrm{t\_off}\right) \land \left(\mathrm{time} \geq \mathrm{t\_on}\right) \\ \begin{cases} \mathrm{A\_max} \cdot \exp\left(\mathrm{alpha} \cdot \left(\mathrm{time} - \mathrm{t\_off}\right)\right) & \text{if time} \geq \mathrm{t\_off} \\ 0 & \text{otherwise} \end{cases} & \text{otherwise} \end{cases} \tag{5}$$

5.6 Rule H1

Rule H1 is a rate rule for parameter H1:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H1} = \left(\mathrm{beta\_I} \cdot \mathrm{H1}\right) + \mathrm{A} \tag{6}$$

5.7 Rule H2

Rule H2 is a rate rule for parameter H2:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H2} = \mathrm{beta\_I} \cdot \mathrm{H1} - \mathrm{beta\_C} \cdot \mathrm{H2} \tag{7}$$

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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