**SBML Model Report**

# Model name: "Mayya2005_STATmodule"

May 5, 2016

## 1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Harish Dharuri[1] at September 26th 2007 at 2:22 a. m. and last time modified at May 27th 2014 at 10:17 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 | 3 |
| species types | 0 | species | 9 |
| events | 0 | constraints | 0 |
| reactions | 7 | function definitions | 0 |
| global parameters | 0 | unit definitions | 9 |
| rules | 1 | initial assignments | 0 |

### Model Notes

The model reproduces Fig 2B of the paper. Model successfully reproduced using MathSBML.



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commercially or not, in a restricted way or not.

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# 2 Unit Definitions

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

## 2.1 Unit substance

**Definition** $\mu\mathrm{mol}$

## 2.2 Unit volume

**Definition** $\mathrm{l}$

## 2.3 Unit area

**Definition** $\mu\mathrm{m}^2$

## 2.4 Unit molecules

**Definition** item

## 2.5 Unit um2

**Definition** $\mu\mathrm{m}^2$

## 2.6 Unit s_1

**Definition** $\mathrm{s}^{-1}$

## 2.7 Unit uM_1_s_1

**Definition** $\mu\mathrm{mol}^{-1} \cdot \mathrm{l} \cdot \mathrm{s}^{-1}$

## 2.8 Unit uM_um_s_1

**Definition** $\mu\mathrm{mol} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{m}^{-2} \cdot \mathrm{s}^{-1}$

### 2.9 Unit uM

**Definition** $\mu mol \cdot l^{-1}$

### 2.10 Unit length

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

**Definition** m

### 2.11 Unit time

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

**Definition** s

## 3 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

| Id | Name | SBO | Spatial Dimensions | Size | Unit | Constant | Outside |
|---|---|---|---|---|---|---|---|
| nuc | nuc | | 3 | 1 | | ☑ | |
| sol | sol | | 3 | 14.625 | | ☑ | |
| nm | nm | | 2 | 1 | $\mu m^2$ | ☑ | |

### 3.1 Compartment nuc

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

**Name** nuc

### 3.2 Compartment sol

This is a three dimensional compartment with a constant size of 14.625 litre.

**Name** sol

### 3.3 Compartment nm

This is a two dimensional compartment with a constant size of one $\mu m^2$.

**Name** nm

## 4 Species

This model contains nine 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 |
|---|---|---|---|---|---|
| `stat_sol` | stat_sol | `sol` | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| `Pstat_sol` | Pstat_sol | `sol` | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| `statKinase_sol` | statKinase_sol | `sol` | $\mu mol \cdot l^{-1}$ | ☐ | ☑ |
| `PstatDimer_sol` | PstatDimer_sol | `sol` | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| `PstatDimer_nuc` | PstatDimer_nuc | `nuc` | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| `stat_nuc` | stat_nuc | `nuc` | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| `Pstat_nuc` | Pstat_nuc | `nuc` | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| `statPhosphatase_nuc` | statPhosphatase_nuc | `nuc` | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |
| `species_test` | species_test | `sol` | $\mu mol \cdot l^{-1}$ | ☐ | ☐ |

# 5 Rule

This is an overview of one rule.

## 5.1 Rule `statKinase_sol`

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

$$\text{statKinase\_sol} = \begin{cases} 0.01 \cdot \sin\left(0.001571 \cdot (-500 + \text{t})\right) & \text{if } (\text{t} > 500) \land (\text{t} < 2502.54614894971) \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

## 6 Reactions

This model contains seven 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 4: Overview of all reactions

| № | Id | Name | Reaction Equation | SBO |
|---|---|---|---|---|
| 1 | PstatDimerisation | PstatDimerisation | $2\,\text{Pstat\_sol} \rightleftharpoons \text{PstatDimer\_sol}$ | |
| 2 | statDephosphorylation | statDephosphorylation | $\text{Pstat\_nuc} \overset{\text{statPhosphatase\_nuc}}{\rightleftharpoons} \text{stat\_nuc}$ | |
| 3 | statPhosphorylation | statPhosphorylation | $\text{stat\_sol} \overset{\text{statKinase\_sol}}{\rightleftharpoons} \text{Pstat\_sol} + \text{species\_test}$ | |
| 4 | PstatDimerisationNuc | PstatDimerisationNuc | $2\,\text{Pstat\_nuc} \rightleftharpoons \text{PstatDimer\_nuc}$ | |
| 5 | PstatDimer_-_import | PstatDimer_ import | $\text{PstatDimer\_sol} \rightleftharpoons \text{PstatDimer\_nuc}$ | |
| 6 | stat_export | stat_export | $\text{stat\_sol} \rightleftharpoons \text{stat\_nuc}$ | |
| 7 | stat_import | stat_import | $\text{stat\_sol} \rightleftharpoons \text{stat\_nuc}$ | |

## 6.1 Reaction PstatDimerisation

This is a reversible reaction of one reactant forming one product.

**Name** PstatDimerisation

### Reaction equation

$$2\,\mathrm{Pstat\_sol} \rightleftharpoons \mathrm{PstatDimer\_sol} \tag{2}$$

### Reactant

Table 5: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| Pstat_sol | Pstat_sol | |

### Product

Table 6: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| PstatDimer_sol | PstatDimer_sol | |

### Kinetic Law

**Derived unit** $10^{-6}\,\mathrm{mol}\cdot\mathrm{s}^{-1}$

$$v_1 = \left(\mathrm{Kf\_PstatDimerisation}\cdot[\mathrm{Pstat\_sol}]^2 + ((\mathrm{Kr\_PstatDimerisation}\cdot[\mathrm{PstatDimer\_sol}]))\right)\cdot\mathrm{vol}\,(\mathrm{sol}) \tag{3}$$

Table 7: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Kf_PstatDimerisation | | | 0.60 | $\mu\mathrm{mol}^{-1}\cdot 1\cdot\mathrm{s}^{-1}$ | ☑ |
| Kr_PstatDimerisation | | | 0.03 | $\mathrm{s}^{-1}$ | ☑ |

## 6.2 Reaction statDephosphorylation

This is a reversible reaction of one reactant forming one product influenced by one modifier.

**Name** statDephosphorylation

### Reaction equation

$$\mathrm{Pstat\_nuc} \xrightleftharpoons{\mathrm{statPhosphatase\_nuc}} \mathrm{stat\_nuc} \tag{4}$$

### Reactant

Table 8: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| Pstat_nuc | Pstat_nuc | |

### Modifier

Table 9: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| statPhosphatase_nuc | statPhosphatase_nuc | |

### Product

Table 10: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| stat_nuc | stat_nuc | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_2 = \mathrm{Kcat\_dephos} \cdot [\mathrm{statPhosphatase\_nuc}] \cdot [\mathrm{Pstat\_nuc}] \cdot \frac{1}{\mathrm{Km\_dephos} + [\mathrm{Pstat\_nuc}]} \cdot \mathrm{vol}\,(\mathrm{nuc}) \tag{5}$$

Table 11: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Kcat_dephos | | | 1.0 | $s^{-1}$ | ☑ |
| Km_dephos | | | 2.0 | $\mu mol \cdot l^{-1}$ | ☑ |

## 6.3 Reaction statPhosphorylation

This is a reversible reaction of one reactant forming two products influenced by one modifier.

**Name** statPhosphorylation

### Reaction equation

$$\text{stat\_sol} \overset{\text{statKinase\_sol}}{\rightleftharpoons} \text{Pstat\_sol} + \text{species\_test} \tag{6}$$

### Reactant

Table 12: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| stat_sol | stat_sol | |

### Modifier

Table 13: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| statKinase_sol | statKinase_sol | |

### Products

Table 14: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| Pstat_sol | Pstat_sol | |
| species_test | species_test | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_3 = \text{Kcat\_phos} \cdot [\text{statKinase\_sol}] \cdot [\text{stat\_sol}] \cdot \frac{1}{\text{Km\_phos} + [\text{stat\_sol}]} \cdot \text{vol}(\text{sol}) \tag{7}$$

Table 15: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Kcat_phos | | | 1.0 | $s^{-1}$ | ☑ |
| Km_phos | | | 4.0 | $\mu mol \cdot l^{-1}$ | ☑ |

## 6.4 Reaction PstatDimerisationNuc

This is a reversible reaction of one reactant forming one product.

**Name** PstatDimerisationNuc

### Reaction equation

$$2\,\text{Pstat\_nuc} \rightleftharpoons \text{PstatDimer\_nuc} \tag{8}$$

### Reactant

Table 16: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| Pstat_nuc | Pstat_nuc | |

### Product

Table 17: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| PstatDimer_nuc | PstatDimer_nuc | |

### Kinetic Law

**Derived unit** $10^{-6}\,\text{mol} \cdot s^{-1}$

$$v_4 = \left(\text{Kf\_PstatDimerisation} \cdot [\text{Pstat\_nuc}]^2 + ((\text{Kr\_PstatDimerisation} \cdot [\text{PstatDimer\_nuc}]))\right) \cdot \text{vol}(\text{nuc}) \tag{9}$$

Table 18: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Kf_PstatDimerisation | | | 0.60 | $\mu mol^{-1} \cdot l \cdot s^{-1}$ | ☑ |
| Kr_PstatDimerisation | | | 0.03 | $s^{-1}$ | ☑ |

## 6.5 Reaction PstatDimer__import

This is a reversible reaction of one reactant forming one product.

**Name** PstatDimer_ import

### Reaction equation

$$\text{PstatDimer\_sol} \rightleftharpoons \text{PstatDimer\_nuc} \tag{10}$$

### Reactant

Table 19: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| PstatDimer_sol | PstatDimer_sol | |

### Product

Table 20: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| PstatDimer_nuc | PstatDimer_nuc | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_5 = \text{PstatDimer\_impMax} \cdot [\text{PstatDimer\_sol}] \cdot \frac{1}{\text{Kpsd\_imp} + [\text{PstatDimer\_sol}]} \cdot \text{area}\,(\text{nm}) \tag{11}$$

Table 21: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| PstatDimer_impMax | | | 0.045 | $\mu mol \cdot l^{-1} \cdot \mu m^{-2} \cdot s^{-1}$ | ☑ |
| Kpsd_imp | | | 0.300 | $\mu mol \cdot l^{-1}$ | ☑ |

## 6.6 Reaction stat_export

This is a reversible reaction of one reactant forming one product.

**Name** stat_export

### Reaction equation

$$\text{stat\_sol} \rightleftharpoons \text{stat\_nuc} \tag{12}$$

### Reactant

Table 22: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| stat_sol | stat_sol | |

### Product

Table 23: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| stat_nuc | stat_nuc | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_6 = \text{vol}(\text{nuc}) \cdot \text{stat\_expMax} \cdot [\text{stat\_nuc}] \cdot \frac{1}{\text{Ks\_exp} + [\text{stat\_nuc}]} \cdot \text{area}(\text{nm}) \tag{13}$$

Table 24: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| stat_expMax | | | −0.06 | $\mu mol \cdot l^{-1} \cdot \mu m^{-2} \cdot s^{-1}$ | ☑ |
| Ks_exp | | | 0.60 | $\mu mol \cdot l^{-1}$ | ☑ |

## 6.7 Reaction stat_import

This is a reversible reaction of one reactant forming one product.

**Name** stat_import

### Reaction equation

$$\text{stat\_sol} \rightleftharpoons \text{stat\_nuc} \tag{14}$$

### Reactant

Table 25: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| stat_sol | stat_sol | |

### Product

Table 26: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| stat_nuc | stat_nuc | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_7 = \text{vol}(\text{nuc}) \cdot \text{stat\_impMax} \cdot [\text{stat\_sol}] \cdot \frac{1}{\text{Ks\_imp} + [\text{stat\_sol}]} \cdot \text{area}(\text{nm}) \tag{15}$$

Table 27: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| stat_impMax | | | 0.003 | $\mu mol \cdot l^{-1} \cdot \mu m^{-2} \cdot s^{-1}$ | ☑ |
| Ks_imp | | | 3.000 | $\mu mol \cdot l^{-1}$ | ☑ |

# 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 stat_sol

**Name** stat_sol

**Initial concentration** $1\ \mu mol \cdot l^{-1}$

This species takes part in three reactions (as a reactant in statPhosphorylation, stat_export, stat_import).

$$\frac{d}{dt}\text{stat\_sol} = -v_3 - v_6 - v_7 \tag{16}$$

## 7.2 Species Pstat_sol

**Name** Pstat_sol

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

This species takes part in two reactions (as a reactant in PstatDimerisation and as a product in statPhosphorylation).

$$\frac{d}{dt}\text{Pstat\_sol} = v_3 - 2v_1 \tag{17}$$

## 7.3 Species statKinase_sol

**Name** statKinase_sol

**Involved in rule** statKinase_sol

This species takes part in one reaction (as a modifier in statPhosphorylation). Not this but one rule determines the species' quantity because this species is on the boundary of the reaction system.

## 7.4 Species PstatDimer_sol

**Name** PstatDimer_sol

**Initial concentration** $0\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in PstatDimer__import and as a product in PstatDimerisation).

$$\frac{\text{d}}{\text{d}t}\text{PstatDimer\_sol} = v_1 - v_5 \tag{18}$$

## 7.5 Species PstatDimer_nuc

**Name** PstatDimer_nuc

**Initial concentration** $0\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a product in PstatDimerisationNuc, PstatDimer__import).

$$\frac{\text{d}}{\text{d}t}\text{PstatDimer\_nuc} = v_4 + v_5 \tag{19}$$

## 7.6 Species stat_nuc

**Name** stat_nuc

**Initial concentration** $0\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a product in statDephosphorylation, stat_export, stat_import).

$$\frac{\text{d}}{\text{d}t}\text{stat\_nuc} = v_2 + v_6 + v_7 \tag{20}$$

## 7.7 Species Pstat_nuc

**Name** Pstat_nuc

**Initial concentration** $0\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in statDephosphorylation, PstatDimerisationNuc).

$$\frac{\text{d}}{\text{d}t}\text{Pstat\_nuc} = -v_2 - 2v_4 \tag{21}$$

## 7.8 Species statPhosphatase_nuc

**Name** statPhosphatase_nuc

**Initial concentration** $0.05\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in statDephosphorylation).

$$\frac{\text{d}}{\text{d}t}\text{statPhosphatase\_nuc} = 0 \tag{22}$$

## 7.9 Species species_test

**Name** species_test

**Initial concentration** $0\ \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{species\_test} = v_3 \tag{23}$$

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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