

## Full Grammer

### Tags and meanings:

\_exc: extracellular;

\_c: intracellular;

METABOLITE: metabolite;

PROTEIN: protein;

MRNA: mRNA;

GENE: gene.

### **Nomenclature** for model generation:

reaction name:

reactant(s)<rxn type:catalyst(s)>product(s)

e.g. 1.0\*p\_MAPK\_c<catalyze:p\_Her2\_ph\_2\_c>1.0\*p\_MAPK\_act\_c

Monod affinity constant in reactions:

MonodK~reaction#~Substrate

e.g. MonodK~rxn4~met\_Testosterone\_c

Weight value in transcriptional control term:

W~actor~target mRNA

e.g. W~p\_MAPK\_act\_c~m\_API\_c

dissociation constant in transfer function:

KD~species name

e.g. KD~p\_AR\_ph\_2\_c

Kinetic equations specification:

Michaelis–Menten Kinetics.

### **Sentence Specification**

Logic AND can be denoted by “and” or comma “,” or “&;”;

Logic OR can be denoted by “or” or “||”.

For clearness and simplicity, the following notations are used:

DS10: a single biological symbol;

E.g. m\_A\_c

DS11: multiple biological symbols linked by logic AND;

E.g. m\_A\_c, m\_D\_C and m\_B\_c

DS1: DS10 or DS11;

DS20: multiple biological symbols linked by logic OR;

E.g. m\_A\_c or m\_D\_C or m\_B\_c

DS21: multiple biological symbol groups linked by logic AND or OR, with each group inside a pair of parentheses if contains multiple biological symbols, only one logic outside parentheses and different logics between inside/outside of parentheses.

E.g. m\_A\_c or m\_D\_C or (m\_B\_c & m\_F\_c)  
m\_A\_c & m\_D\_C & (m\_B\_c or m\_F\_c)

DS22: multiple biological symbol groups linked by logic AND or OR, with every group contains multiple biological symbols, only one logic outside parentheses and different logics between inside/outside of parentheses.

E.g. (m\_A\_c and m\_E\_c) or (m\_G\_c and m\_D\_C) or (m\_B\_c & m\_F\_c)  
(m\_A\_c || m\_E\_c) & (m\_G\_c or m\_D\_C) and (m\_B\_c || m\_F\_c)

DS2: DS20 or DS21 or DS22;

**Is:**

DS10 is/was DS10

DS11 are/were DS11

**React:**

In default it is reversible, add “irreversibly” to change it.

DS1 reacts/ reacted/ reacting/ react into []

[] reacts/ reacted/ reacting/ react into DS1

**Uptake:**

In default it is irreversible, add “reversibly” to change it.

The cell uptake/ uptakes/ uptaking/ uptook DS10

The cell uptake/ uptakes/ uptaking/ uptook DS11

The cell uptake/ uptakes/ uptaking/ uptook DS10 via/through DS10

The cell uptake/ uptakes/ uptaking/ uptook DS10 via/through DS11

**Secrete:**

In default it is irreversible, add “reversibly” to change it.

The cell secrete/ secretes/ secreted/ secreting DS10

The cell secrete/ secretes/ secreted/ secreting DS11

The cell secrete/ secretes/ secreted/ secreting DS10 via/through DS10

The cell secrete/ secretes/ secreted/ secreting DS10 via/through DS11

**Bind:**

In default it is reversible, add “irreversibly” to change it.

DS1 bind/ binding/ bound/ binds

DS1 associate/ associates/ associated/ associating

DS1 complex/ complexes/ complexed/ complexing

DS1 bind/ binding/ bound/ binds into DS10

DS1 associate/ associates/ associated/ associating into DS10  
DS1 complex/ complexes/ complexed/ complexing into DS10

### **Unbind:**

In default it is reversible, add “irreversibly” to change it.  
DS10 unbind/ unbinds/ unbound/ unbinding/ dissociate/ dissociates/ dissociated/  
dissociating  
DS10 unbind/ unbinds/ unbound/ unbinding/ dissociate/ dissociates/ dissociated/  
dissociating into DS1

### **Phosphorylation:**

In default it is irreversible, add “reversibly” to change it.  
DS1 phosphorylate/ phosphorylates/ phosphorylated/ phosphorylating DS10  
DS2 phosphorylate/ phosphorylates/ phosphorylated/ phosphorylating DS10  
DS1 phosphorylate/ phosphorylates/ phosphorylated/ phosphorylating DS10 at site DS10  
DS2 phosphorylate/ phosphorylates/ phosphorylated/ phosphorylating DS10 at site DS10

### **Dephosphorylation:**

In default it is irreversible, add “reversibly” to change it.  
DS1 dephosphorylate/ dephosphorylates/ dephosphorylated/ dephosphorylating DS10  
DS2 dephosphorylate/ dephosphorylates/ dephosphorylated/ dephosphorylating DS10  
DS1 dephosphorylate/ dephosphorylates/ dephosphorylated/ dephosphorylating DS10 at  
site DS10  
DS2 dephosphorylate/ dephosphorylates/ dephosphorylated/ dephosphorylating DS10 at  
site DS10

### **Activation:**

In default it is irreversible, add “reversibly” to change it.  
DS1 activate/ activates/ activating/ activated the expression/ transcription/ translation of  
DS1  
DS1 promote/ promotes/ promoting/ promoted the expression/ transcription/ translation  
of DS1  
DS1 induce/ induces/ inducing/ induced the expression/ transcription/ translation of DS1  
DS1 upregulate/ upregulates/ upregulated/ upregulating the expression/ transcription/  
translation of DS1  
DS2 activate/ activates/ activating/ activated the expression/ transcription/ translation of  
DS1  
DS2 promote/ promotes/ promoting/ promoted the expression/ transcription/ translation  
of DS1  
DS2 induce/ induces/ inducing/ induced the expression/ transcription/ translation of DS1

DS2 upregulate/ upregulates/ upregulated/ upregulating the expression/ transcription/ translation of DS1

Note: **induce** acts on GENE, and **activate** on enzyme.

### **Inhibition:**

In default it is irreversible, add “reversibly” to change it.

DS1 inhibit/ inhibits/ inhibiting/ inhibited the expression/ transcription/ translation of DS1

DS1 repress/ represses/ repressing/ repressed the expression/ transcription/ translation of DS1

DS1 downregulate/ downregulates/ downregulated/ downregulating the expression/ transcription/ translation of DS1

DS2 inhibit/ inhibits/ inhibiting/ inhibited the expression/ transcription/ translation of DS1

DS2 repress/ represses/ repressing/ repressed the expression/ transcription/ translation of DS1

DS2 downregulate/ downregulates/ downregulated/ downregulating the expression/ transcription/ translation of DS1

Note: **repress** acts on GENE, and **inhibit** on enzyme.

### **Catalyze:**

In default it is irreversible, add “reversibly” to change it.

DS1 catalyze/ catalyzes/ catalyzed/ catalyzing the (reversible) conversion of DS1 into DS1

DS1 catalyse/ catalyses/ catalysed/ catalysing the (reversible) conversion of DS1 into DS1

DS2 catalyze/ catalyzes/ catalyzed/ catalyzing the (reversible) conversion of DS1 into DS1

DS2 catalyse/ catalyses/ catalysed/ catalysing the (reversible) conversion of DS1 into DS1

### **Semantic error checking:**

In “react” type, one of two symbols should be “[ ]”.

In “uptake” type, membrane transporters can only be of type “PROTEIN”.

In “secrete” type, the cell can only secrete species of type “METABOLITE” or “PROTEIN”, and membrane transporters can only be of type “PROTEIN”.

In “bind” type, “GENE” can not bind with “GENE”, and the binding complex can’t be “GENE”.

In “unbind” type, a complex of “GENE” type is not allowed.

In “phosphorylation” type, the enzyme is of type “PROTEIN” or is “[ ]” if no enzyme participates in the reaction. Only “PROTEIN” can be phosphorylated.

In “dephosphorylation” type, the enzyme is of type “PROTEIN” or is “[]” if no enzyme participates in the reaction. Only “PROTEIN” can be dephosphorylated.

In “catalyze” type, enzymes are “PROTEIN”, reactants/products can be “METABOLITE” and/or “PROTEIN” and/or “GENE”.

In “activation” type, regulators can only be “PROTEIN” and/or “METABOLITE”.

In “inhibition” type, regulators can only be “PROTEIN” and/or “METABOLITE”.

“#” is reserved for inline comments.