

Full Grammer

Tags and meanings:

_exc: extracellular;

_c: intracellular;

METABOLITE: metabolite;

PROTEIN: protein;

MRNA: mRNA;

GENE: gene;

-pho: phosphorylated compound.

Note: specifying _exc, _c, METABOLITE, PROTEIN and MRNA is a hard requirement for all descriptions.

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_AP1_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

Note: the name of the uptake compound is derived from the compound, for example (assume the user claims “_e, _c are _exc, _c”): “the cell uptakes **m_A_e**” will generate product as “**m_A_c**”.

The user can refer to the product in her/his following description.

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

Note: the name of the secrete compound is derived from the compound, for example (assume the user claims “_e, _c are _exc, _c”): “the cell secretes **m_C_c**” will generate product as “**m_C_e**”.

The user can refer to the product in her/his following description.

Bind:

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

DS11 bind/ binding/ bound/ binds

DS11 associate/ associates/ associated/ associating

DS11 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

Note: the name of the bind compound, if not specified, is generated by linking reactants' names together by "--", for example: "p_E4_c and p_E5_c binding" will generate product as "p_E4_c--p_E5_c". The user can refer to the product in her/his following description.

Unbind:

In default it is reversible, add "irreversibly" to change it.

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

Note: the name of the phosphorylated compound is derived from the compound, for example (assume the user claims "-phos is -pho"):

"p_E1_c phosphorylates p_E2_c" will generate product as "p_E2_c-phos";

"p_E1_c phosphorylates p_E2_c at site xyz" will generate product as "p_E2_c-xyz" since the site is specified here.

The user can refer to the product, as "p_E2_c-phos" and "p_E2_c-xyz" respectively in the first and second example, in her/his following description.

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

Note: the name of the dephosphorylated compound is derived from the compound, for example (assume the user claims "-phos is -pho"):

"p_E3_c dephosphorylate p_E2_c-phos" will generate product as "p_E2_c";

"p_E4_c dephosphorylate p_E2_c-xyz at site xyz" will generate product as "p_E2_c".

The user can refer to the product, as "p_E2_c" and "p_E2_c" respectively in the first and second example, in her/his following description.

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”.