

# CADLIVE Text Editor Ver.2.15

## A table of contents

1. TextEditor.....	1
2. Operating environment.....	1
3. Startup .....	1
3.1 Start of TextEditor .....	1
4. Creation of a new model .....	2
4.1 Model creation.....	2
4.1.1 Creation of a new model.....	2
4.1.2 EntryModel.....	2
5. Registration of compartment.....	3
5.1 Registration of compartment .....	3
5.1.1 ReactionList.....	4
5.2 Edition of compartment volume.....	4
6. Explanation of specie list .....	5
6.1 Specie list .....	5
6.1.1 SpecieList spreadsheet.....	5
6.1.2 Compartment tab .....	5
6.1.3 AddSpecie button.....	5
6.1.4 ReactionList button.....	5
7. Registration and edition of species.....	6
7.1 Registration of species.....	6
7.1.1 New registration of a species.....	6
7.1.2 Screen for registering a specie.....	7
7.2 Species edition.....	9
7.2.1 Edition of a species.....	9
7.2.2 Species edition.....	10
8. Explanation of screen for listing reactions.....	12
8.1 Switching the screen mode for listing reactions .....	12
8.1.1 All mode .....	12
8.1.2 Convertible mode .....	12
8.2 Explanation of screen for listing reactions .....	12
8.2.1 ReactionList spreadsheet .....	12
8.2.2 Layer tab .....	13
8.2.3 AddReaction button .....	13
8.2.4 SpecieList button .....	13
9. Registration and edition of reaction .....	13
9.1 Registration of reaction .....	13
9.1.1 Registration of a new reaction .....	13
9.1.2 Registration of reaction (All mode) .....	14
9.1.3 Registration of reaction (Convertible mode) .....	16
9.2 Edition of reaction .....	17
9.2.1 Edition of reaction .....	17

9.2.2 Edition of reaction (All mode) .....	18
9.2.3 Edition of reaction (Convertible mode) .....	19
10. Merge Function .....	20
10.1 Merge.....	20
11.Explanation of menu items.....	20
11.1 File menu .....	20
11.1.1 New.....	21
11.1.2 Open.....	21
11.1.3 Merge.....	21
11.1.4 Save.....	21
11.1.5 SaveAs .....	21
11.1.6 Exit.....	22
11.2 VIEW menu .....	22
11.3 HELP menu .....	22
11.3.1 AboutTextEditor.....	22

Notice:

There are two kinds of CADLIVE editors: the GUI editor and text editor. Users are recommended to draw a large-scale biochemical network by using the GUI editor and to elaborately edit the generated regulator-reaction equations by using the text editor. The text editor handles the XML file created by the GUI editor, but the GUI editor cannot read the XML file edited by the text editor.

## 1.TextEditor

This editor constructs a concrete biochemical network in the sanac format, which is the extension from SBML (Systems Biology Markup Language), by input of strings and by choosing items on the spreadsheet. This editor can read the sanac files that have been edited by the CADLIVE GUI editor, and writes the sanac files necessary for the simulator of CADLIVE.

## 2. Operating environment

Hardware:

CPU : Pentium3 500MH z or higher  
Memory : >64MB (>256MB is recommended)  
HDD : >1Gb

Software

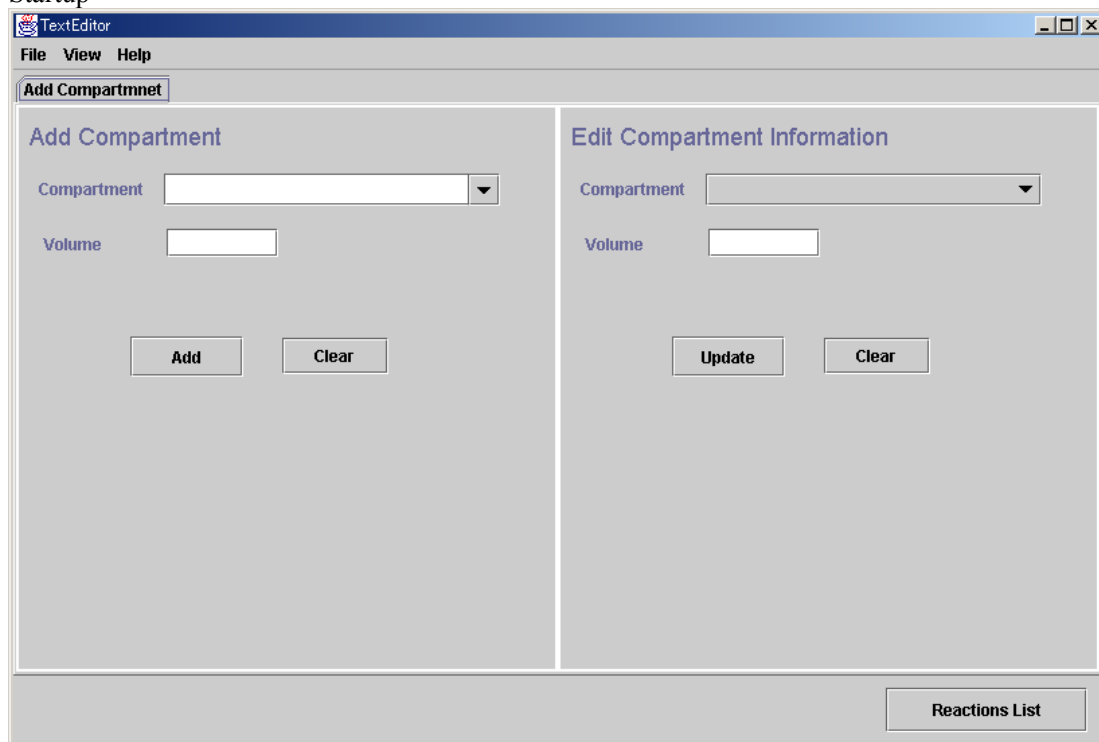
Windows 98、NT4.0、2000、XP  
Java™ 2 Runtime Environment (1.3 is recommended)

## 3. Startup

### 3.1 Start of TextEditor

Java™ 2 Runtime Environment (1.3 is recommended) is required. Start by choosing the [TEXTEDITOR] menu from the program menu.

Startup



## 4. Creation of a new model

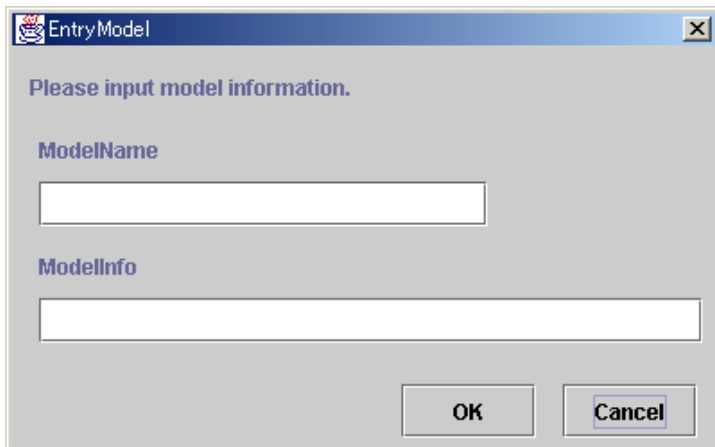
### 4.1 Model creation

#### 4.1.1 Creation of a new model



Click [File] and select [New].

#### 4.1.2 EntryModel



Input "ModelName". If necessary, input "ModelInfo".

Clicking the [OK] button displays the screen for editing a network.  
The button of [Cancel] cancels the entry model.

\* When the [OK] button is clicked without inputting ModelName, warning is given.

## 5. Registration of compartment

### 5.1 Registration of compartment

The screenshot shows a software window titled 'TextEditor' with a menu bar (File, View, Help) and a tab labeled 'Add Compartment'. The main area is divided into two panels. The left panel, titled 'Add Compartment', contains a 'Compartment' dropdown menu, a 'Volume' text input field, and 'Add' and 'Clear' buttons. The right panel, titled 'Edit Compartment Information', contains a 'Compartment' dropdown menu, a 'Volume' text input field, and 'Update' and 'Clear' buttons. At the bottom right of the window is a button labeled 'Reactions List'.

In the screen for the specie list, clicking the [AddCompartment] tab opens the screen for registering the compartment. The tab of [Add Compartment] sets "Compartment", the tab of [Edit Compartment] edits the existing information regarding the compartment. Users select the compartment name from the selectbox or input it manually. If necessary, input "Volume".

This screenshot shows a close-up of the 'Add Compartment' interface. It features three tabs at the top: 'Add Compartment', 'cytoplasm', and 'environment'. The 'Add Compartment' tab is active, showing the 'Compartment' dropdown menu, the 'Volume' text input field, and the 'Add' and 'Clear' buttons.

Following the input, clicking the [Add] button registers "Compartment".

Clicking the [Clear] button resets input data.

\* The added compartment is deleted from the selectbox.

When "Compartment" is missed, clicking the [Add] button displays the error as follows.



#### 5.1.1 ReactionList

To make new reactions or to refer to the list of reactions, click the [ReactionList] button; the screen for the reaction list appears.

#### 5.2 Edition of compartment volume

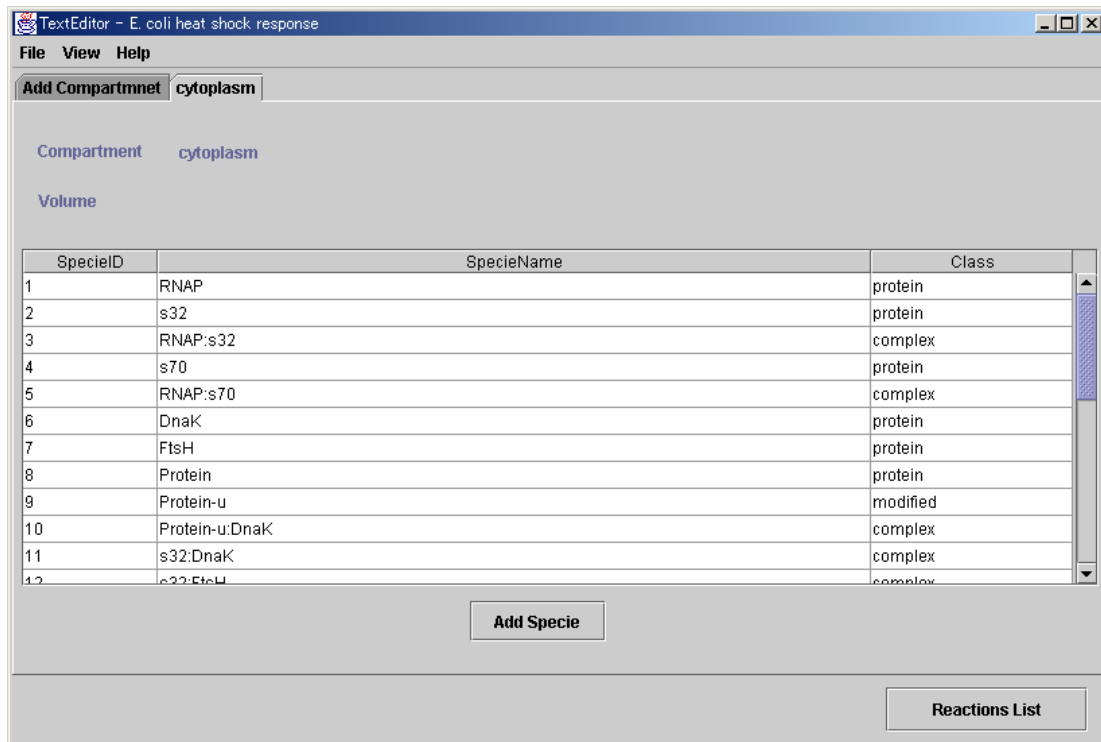
A dialog box titled 'Edit Compartment Information' in blue text. It has a light gray background. There are two main input areas: 'Compartment' with a dropdown menu and 'Volume' with a text input field. At the bottom, there are two buttons: 'Update' and 'Clear'.

Select "Compartment", whose volume users want to change, from the selectbox, and input "Volume". Clicking the [Update] button updates the volume of the selected compartment.

\* The selectbox shows the registered compartments.

## 6. Explanation of specie list

### 6.1 Specie list



#### 6.1.1 SpecieList spreadsheet

The registered species are listed every compartment. Double clicking the specie on the spreadsheet displays the window for editing a specie.

#### 6.1.2 Compartment tab

The compartment tab shows the compartment that the specie belongs. Clicking the tab displays the list of the species located in the compartment. The tab of "AddCompartment" registers a new compartment.

#### 6.1.3 AddSpecie button

This button registers a new species. Open the compartment tab, and click the [AddSpecie] button. The screen for registering species will be displayed.

#### 6.1.4 ReactionList button

To make new reactions, or to refer to the list of reactions, click the [ReactionList] button. The screen for listing reactions is displayed.

## 7. Registration and edition of species

### 7.1 Registration of species

#### 7.1.1 New registration of a species

The screenshot shows a software window titled "E. coli heat shock response". It has a menu bar with "File", "View", and "Help". Below the menu bar are three tabs: "Add Compartment", "cytoplasm", and "environment". The "environment" tab is currently selected. Inside the window, there are labels for "Compartment" (with "environment" selected), "Volume", and a table for species registration. The table has three columns: "SpecieID", "SpecieName", and "Class". Below the table is an "Add Specie" button. At the bottom right of the window is a "Reactions List" button.

SpecieID	SpecieName	Class
----------	------------	-------

**Add Specie**

**Reactions List**

Open the "Compartment" tab of interest, and click the [AddSpecie] button. The screen for registering a species is displayed.

### 7.1.2 Screen for registering a specie

SpecieID 32

SpecieName

Compartment **environment**

Class

TotalAmount ☒ variable ☐ constant

MassBalance ☒ on ☐ off

Decomposition ☒ on ☐ off

InitialAmount

List Of Elements

SpecieName	Compartment	stoichiometry

Add Cancel

- SpecieID

The system gives "SpecieID" automatically. (Users are not allowed to edit it.)

- SpecieName

Name the specie arbitrarily.

- Compartment

Choose the compartment from the selectbox

- Class

Choose the class from the selectbox. Selection of the class sets the attribute of "TotalAmount", "MassBalance", and "Decomposition" as default values as follows.

- Default value

SpecieClass	TotalAmount	MassBalance	Decomposition
DNA_gene	constant	off	off
DNA_promoter	constant	on	off
DNA_enhancer	constant	on	off
DNA_others	constant	on	off

RNA	variable	off	on
protein	variable	on	on
metabolite	constant	off	off
environmental_factor	constant	off	off
ion_signal	constant	off	off
complex	variable	off	on
modified	variable	on	on
others	constant	off	off
small_molecule	constant	off	off
text_option	constant	off	off

- TotalAmount

Choose the attribute of "TotalAmount" with the radiobutton.

- MassBalance

Choose the attribute of "MassBalance" with the radiobutton.

- Decomposition

Choose the attribute of "Decomposition" with the radiobutton.

- InitialAmount

If necessary, set a numerical value to "InitialAmount".

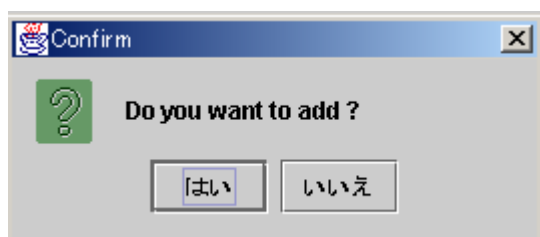
- ListOfElements

The elements are selected from the selectbox.

\* The selectbox has the registered species.

\* Users can delete the input data by choosing [Delete] in the selectbox.

After setting, click the [Add] button to display the confirmation screen. If there is no problem, click [Yes] to register the specie.



Click the [Cancel] button to abandon the registration.

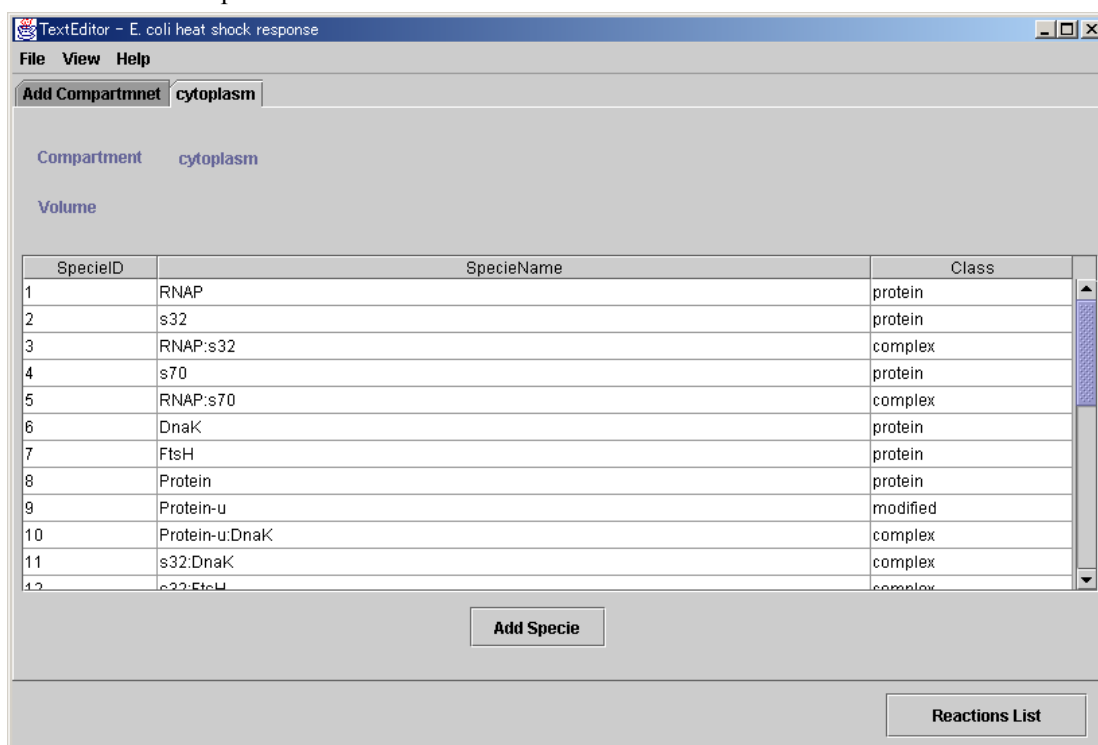
\* When the item for input is shortage or required to reedit, the following warning appears.

Click the [OK] button, and set the items again.



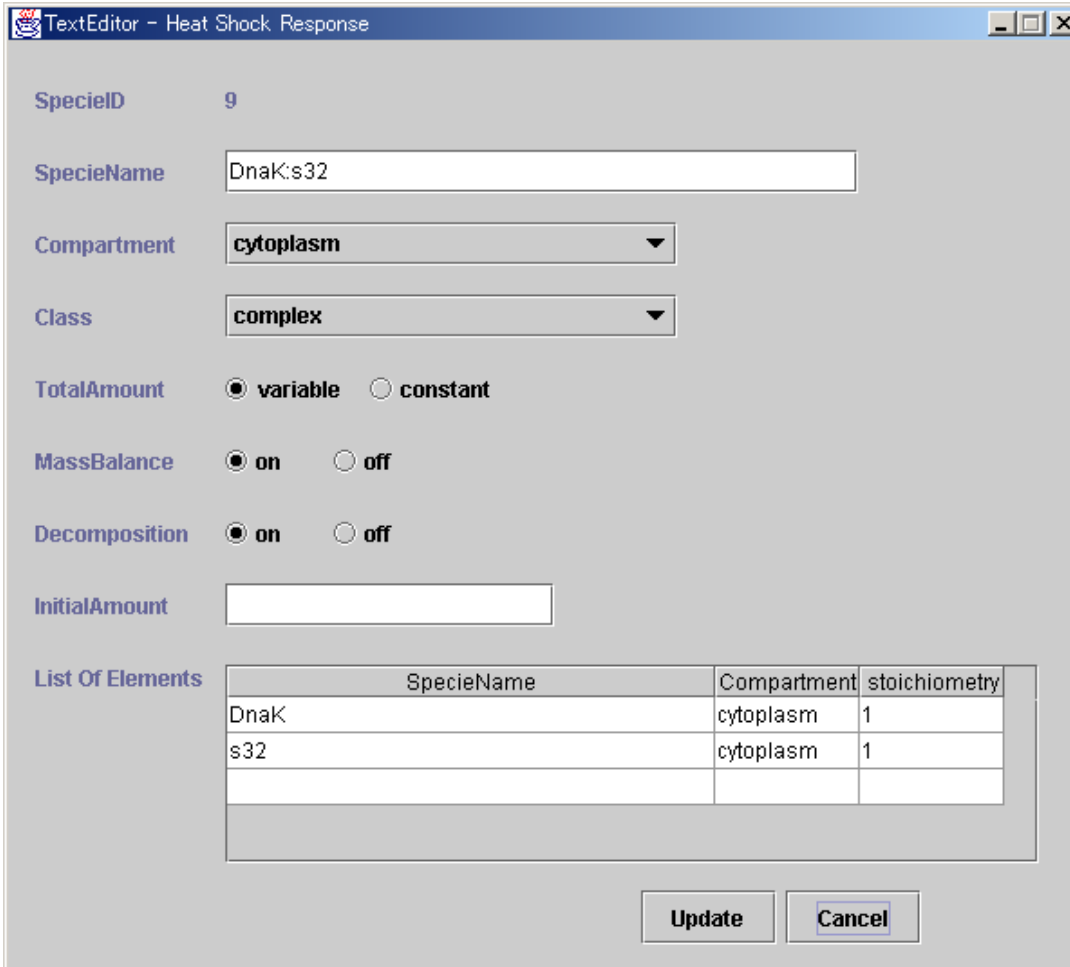
## 7.2 Species edition

### 7.2.1 Edition of a species



In the screen for listing the species, double clicking the species that users want to edit displays the window for editing a species.

## 7.2.2 Species edition



**SpeciesID** 9

**SpecieName** DnaK:s32

**Compartment** cytoplasm

**Class** complex

**TotalAmount** ☒ variable ☐ constant

**MassBalance** ☒ on ☐ off

**Decomposition** ☒ on ☐ off

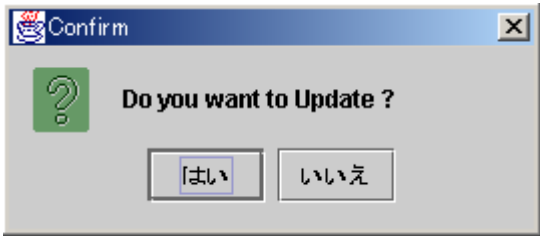
**InitialAmount**

**List Of Elements**

SpecieName	Compartment	stoichiometry
DnaK	cytoplasm	1
s32	cytoplasm	1

**Update** **Cancel**

The edition is carried out in the same manner as the registration of a new species. After setting is completed, clicking the [Update] button displays the confirmation window. If there is no problem, click [YES] to update the data.



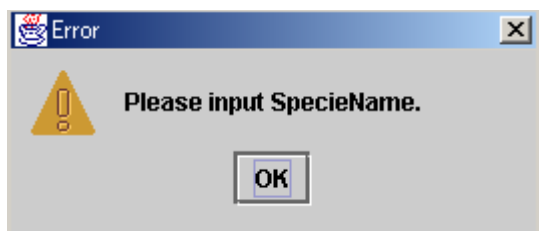
**Confirm**

Do you want to Update ?

**はい** **いいえ**

Click the [Cancel] button to abandon the registration.

\* When the item for input is shortage or required to reedit, the following warning appears. Click the [OK] button, and set the items again.



\* When the attribute of "Class" of the species is "ModifierComplex", the attributes of "SpecieName", "Compartment", "Class", and "ListOfElements" are not allowed to edit.

TextEditor - E. coli heat shock response

SpecieID: 32

SpecieName: s32:RNAP:s32

Compartment: cytoplasm

Class: modifier\_complex

TotalAmount: ☒ variable ☐ constant

MassBalance: ☐ on ☒ off

Decomposition: ☐ on ☒ off

InitialAmount:

List Of Elements

SpecieName	Compartment	stoichiometry
s32	cytoplasm	1

Update Cancel

## 8. Explanation of screen for listing reactions

### 8.1 Switching the screen mode for listing reactions



#### 8.1.1 All mode

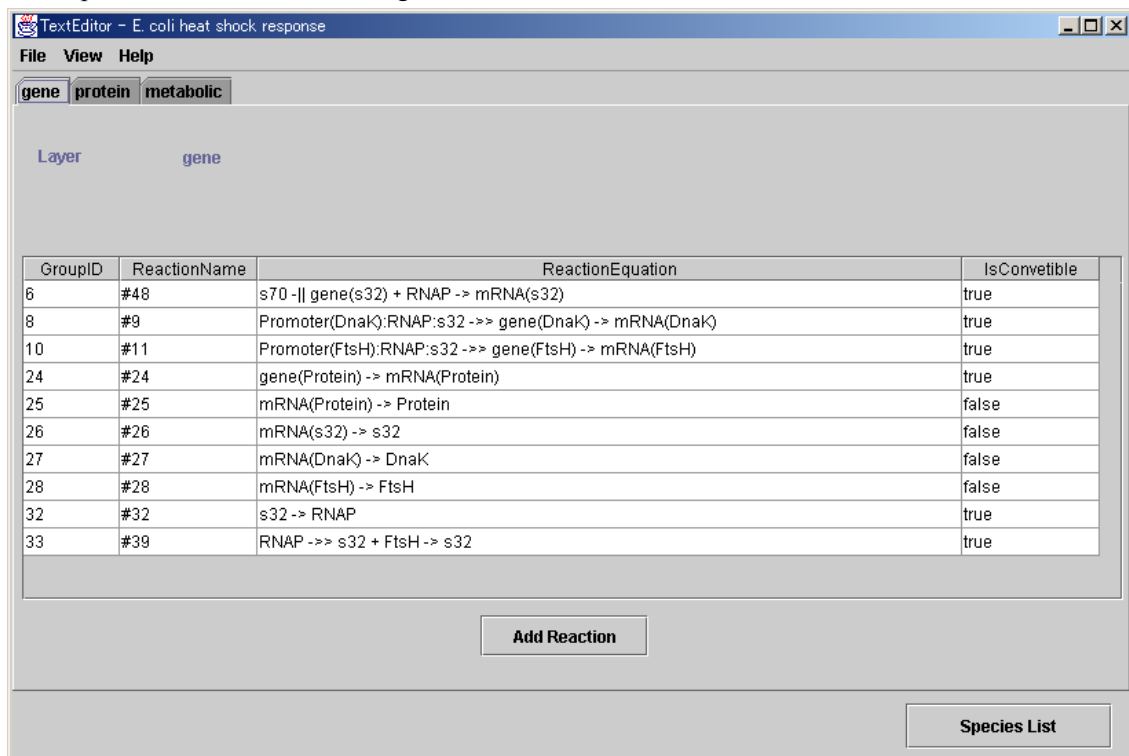
All the reactions are listed despite the value of "isConvertible".

#### 8.1.2 Convertible mode

The reactions with the attribute "isConvertible = true" are listed.

\* For multiple reactions with the same "GroupID", they are not listed on the spreadsheet, when they contain a reaction with attribute "isConvertible = false".

### 8.2 Explanation of screen for listing reactions



#### 8.2.1 ReactionList spreadsheet

The registered reactions are listed every layer. Double clicking the reaction on the spreadsheet displays the window for editing reactions.

### 8.2.2 Layer tab

The "Layer" tab indicates the layer that reactions belong to. Clicking the layer tab displays the list of reactions every layer.

### 8.2.3 AddReaction button

The [AddReaction] button is clicked to create a new reaction.

Open the "Layer" tab, and display the screen for registering a reaction.

\* When "All" mode has been selected, reactions are added separately.

On the other hand, when "Convertible" mode has been selected, the reactions with the same "GroupID" are edited at the same time.

### 8.2.4 SpecieList button

Click the [SpecieList] button to edit a new species or to refer to the list of species. The screen for listing species appears.

## 9. Registration and edition of reaction

### 9.1 Registration of reaction

#### 9.1.1 Registration of a new reaction

The screenshot shows a window titled "E. coli heat shock response" with a menu bar (File, View, Help) and three tabs: "gene", "protein", and "metabolic". The "metabolic" tab is selected, and the "Layer" dropdown menu is set to "metabolic". Below the tabs is a table with the following columns: "GroupID", "ReactionName", "ReactionEquation", and "IsConvettible". The table is currently empty. At the bottom of the window, there are two buttons: "Add Reaction" and "Species List".

GroupID	ReactionName	ReactionEquation	IsConvettible
---------	--------------	------------------	---------------

Click the "Layer" tab and click the [AddReaction] button, the screen for registering reactions is displayed.

\* When "All" mode has been selected, reactions are added separately. On the other hand, when "Convertible" mode has been selected, the reactions with the same "GroupID" are edited at the same time.

### 9.1.2 Registration of reaction (All mode)

ReactionID

Layer: protein

reactionType: [dropdown]

IsConvertible: ☐ true ☒ false

List of Modifier

SpecieName	Compartment	modifierType	isTotal

List of Reactants

SpecieName	Compartment	stoichiometry

ModifierComplex

SpecieName	Compartment

List of Products

SpecieName	Compartment	stoichiometry

ReactionEquation

[Delete] [Add] [Cancel]

- ReactionID

The system gives the “reactionID” to the reaction automatically. (Users are not allowed to edit.)

- Layer

The “Layer” shows the layer that has been selected on the screen for listing reactions.

- reactionType

Choose “reactionType” from the selectbox.

When “reactionType” is selected, the examples are illustrated in the white box on the right as follows.

```
cf.gene(A) -> mRNA(A)
Promoter(A):Repressor-||gene(A) -> mRNA(A)
Enhancer(A):Activator->> gene(A) -> mRNA(A)
```

- isCovertible

This attribute determines if the reaction is converted or not to a mathematical model by the CADLIVE Simulator.

false: not converted  
true: converted.

- ListOfModifier

In order to register a regulator (modifier), the species is selected as “Modifier” from the selectbox.

- modifierType

The attribute of “modifierType” is selected from the selectbox.

- isTotal

The attribute of “isTotal” is selected from the selectbox.

- ListOfReactants

The species are selected as reactants from the selectbox.

\* The selectbox registers the species, but it registers the reaction when “ReactionType “ is “activation\_of\_modifier”, or “inhibition\_of\_modifier”.

\* Users can delete the input data by choosing [Delete] in the selectbox.

- ModifierComplex

When “modifierType = enzyme”, choosing the element of “ListOfModifier” and “ListOfReactants” automatically produces the element of “ModifierComplex”.

- ListOfProducts

The species are selected as products from the selectbox.

\* The selectbox has the registered species.

\* Users can delete the input data by choosing [Delete] in the selectbox.

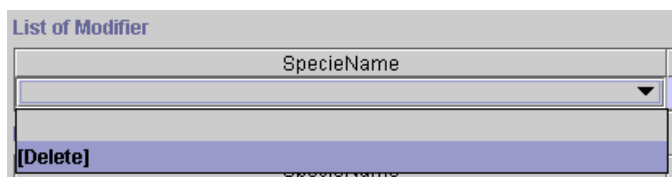
- ReactionEquation

The ReactionEquation is automatically generated. It is ModifierReactionEquation.

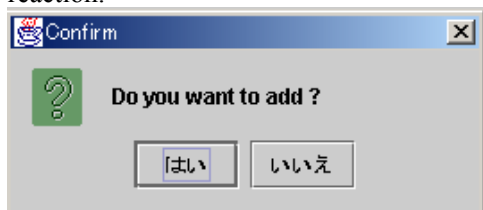
- Stoichiometry

If necessary, click the cell to input a numerical number.

Pushing the [Enter] key decides the stoichiometry.

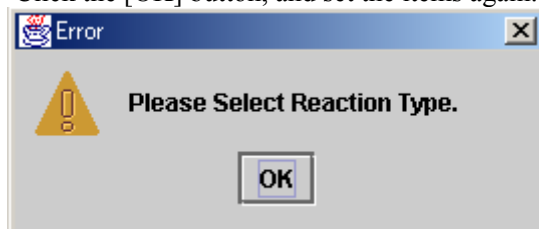


After the setting, click the [Add] button to show the confirmation screen. Clicking [YES] to add the reaction.



To abandon the registration, click the [Cancel] button.

\*When the item for input is shortage or required to reedit, the following warning appears. Click the [OK] button, and set the items again.



### 9.1.3 Registration of reaction (Convertible mode)

TextEditor - E. coli heat shock response

Layer:

IsConvertible: ☒ true ☐ false

ReactionType:

List of Modifier

SpecieName	Compartment	modifierType	isTotal

List of Reactants

Specie/Reaction	Compartment/Layer	stoichiometry

Modifier Complex

SpecieName	Compartment

List of Products

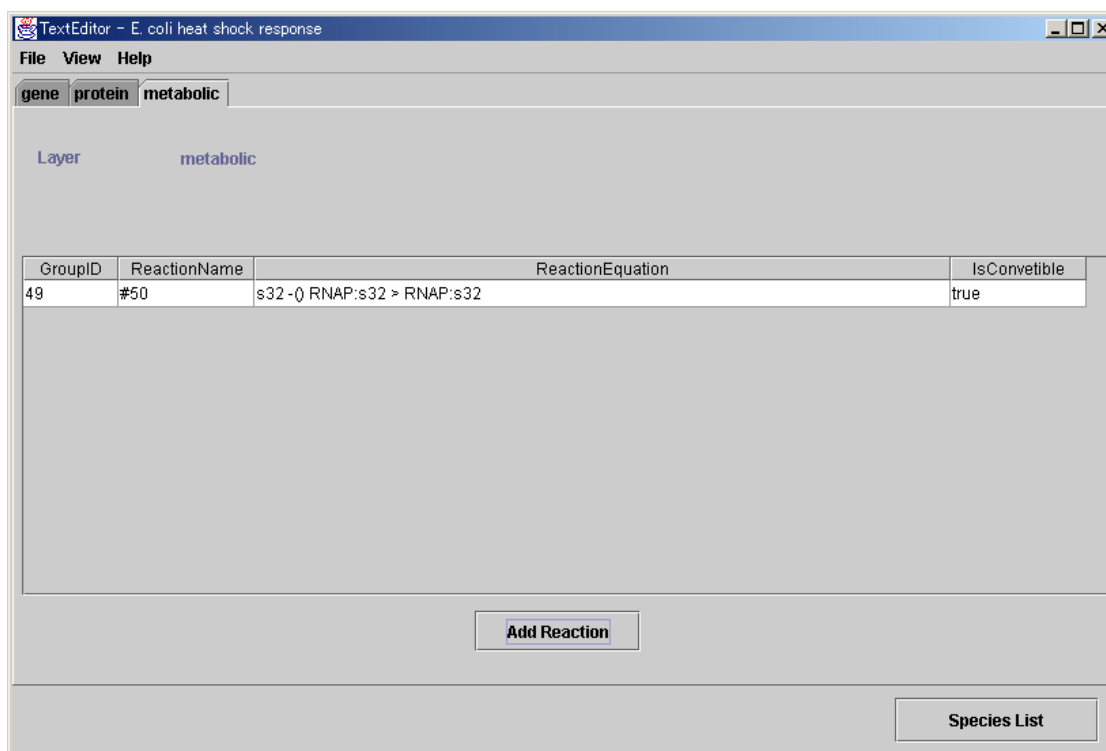
SpecieName	Compartment	stoichiometry

ReactionEquation

In the “Convertible” mode, mutiple regulators (modifiers) are selected with respect to a specific reaction (“ListOfReactants” and “ListOfProducts”). These regulator-reaction equations are given the common “GroupID”.

## 9.2 Edition of reaction

### 9.2.1 Edition of reaction



On the screen for listing reactions, double clicking the reaction displays the window for editing a reaction.

\* When "All" mode has been selected from "View", reactions are added separately. On the other hand, when "Convertible" mode has been selected, the reactions with the same "GroupID" are edited at the same time.

### 9.2.2 Edition of reaction (All mode)

TextEditor - Heat Shock Response

ReactionID: 1

Layer: protein

reactionType: binding

IsConvertible: ☒ true ☐ false

List of Modifier

SpecieName	Compartment	modifierType	isTotal

List of Reactants

SpecieName	Compartment	stoichiometry
RNAP	cytoplasm	1
s70	cytoplasm	1

ModifierComplex

SpecieName	Compartment

List of Products

SpecieName	Compartment	stoichiometry
RNAP:s70	cytoplasm	1

ReactionEquation

RNAP + s70 <=> RNAP:s70

Delete Update Cancel

The edition is carried out in the same manner as the registration of the reactions. After setting, click the [Update] button to show the confirmation screen. Click [YES] to update the revision. To reedit, click [NO].

Confirm

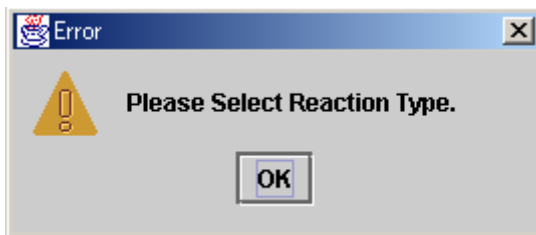
Do you want to Update ?

☒ はい ☐ いいえ

Click the [Cancel] button to abandon the registration.

Click the [Delete] button to delete the reaction.

\* When the item for input is shortage or required to reedit, the following warning appears. Click the [OK] button, and set the items again.



### 9.2.3 Edition of reaction (Convertible mode)

TextEditor - E. coli heat shock response

Layer:

IsConvertible: ☒ true ☐ false

ReactionType:

cf.  
A + B > A-B  
E -() A + B > A-B

List of Modifier

SpecieName	Compartment	modifierType	isTotal
DnaK	cytoplasm	enzyme	true
s70	cytoplasm	enzyme	true

List of Reactants

Specie/Reaction	Compartment/Layer	stoichiometry
RNAP	cytoplasm	1

ModifierComplex

SpecieName	Compartment
DnaK:RNAP	cytoplasm
s70:RNAP	cytoplasm

List of Products

SpecieName	Compartment	stoichiometry
RNAP	cytoplasm	1

ReactionEquation

DnaK-() RNAP > RNAP  
s70-() RNAP > RNAP

Delete Update Cancel

The reactions with the same “GroupID” are edited together. When the “Convertible” mode has been selected, multiple regulators (modifiers) can be selected. In the other respects, “Convertible” mode is the same as “All” mode.

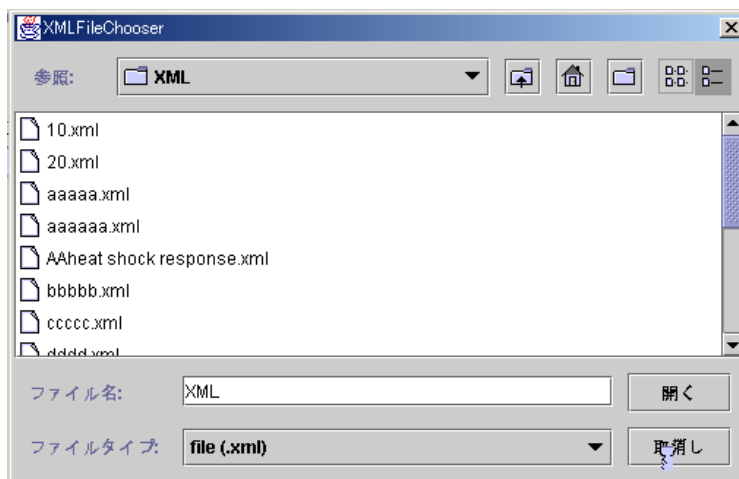
\*The reactions with “IsConvertible = false” are omitted from the list on the “Convertible” mode, but the “All” mode displays all the reactions despite the value of “IsConvertible”.

## 10. Merge Function

### 10.1 Merge



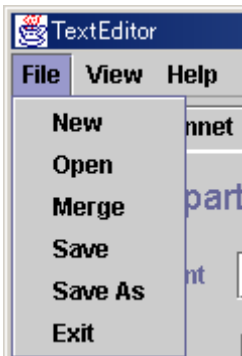
In order to merge the existing network into the current network, choose [Merge] from the "File" menu and select the sanac file to be merged.



\* The model name, comments, and data regarding visualization of a network to be merged are omitted, and integrated into the current model.

## 11.Explanation of menu items

### 11.1 File menu



#### 11.1.1 New

A new model is created.

#### 11.1.2 Open

An existing sanac file is opened

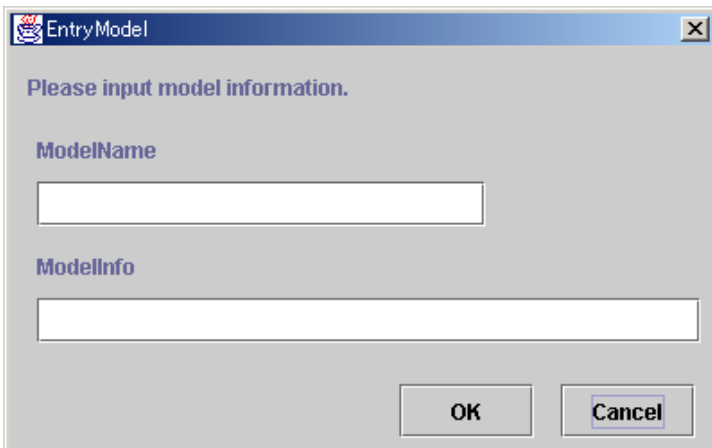
#### 11.1.3 Merge

An existing file is merged into the current file.

#### 11.1.4 Save

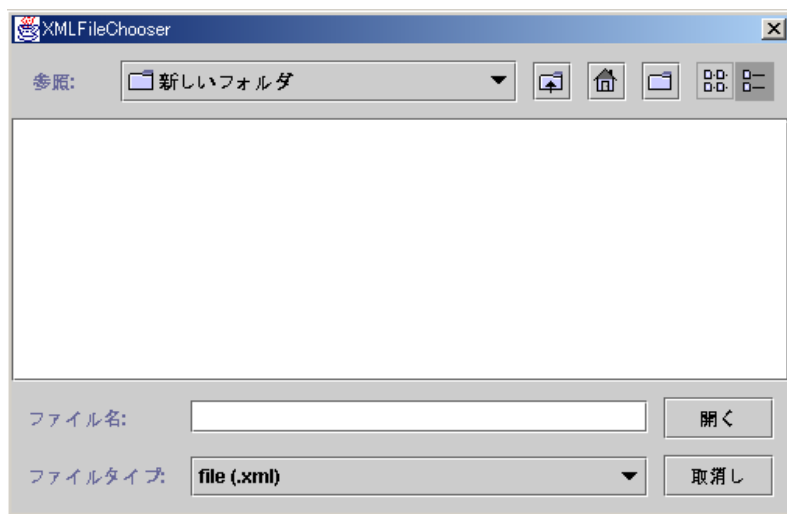
The current network overwrites the existing one, and is saved.

\* When saving a file without "ModelName", the window for setting "ModelName" appears. Input "ModelName", if necessary, "ModelInfo".



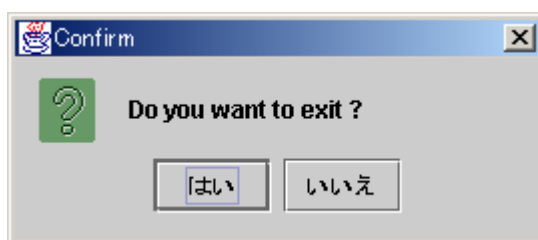
#### 11.1.5 SaveAs

The current file is named and saved.



### 11.1.6 Exit

Finishing the editor.



## 11.2 VIEW menu



Switching the view mode.

## 11.3 HELP menu

### 11.3.1 AboutTextEditor



The version of the TextEditor is displayed.