

CADLIVE Text Editor Ver.2.15

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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 500MHz or higher
Memory : >64MB (>256MB is recommended)
HDD : >1Gb

Software

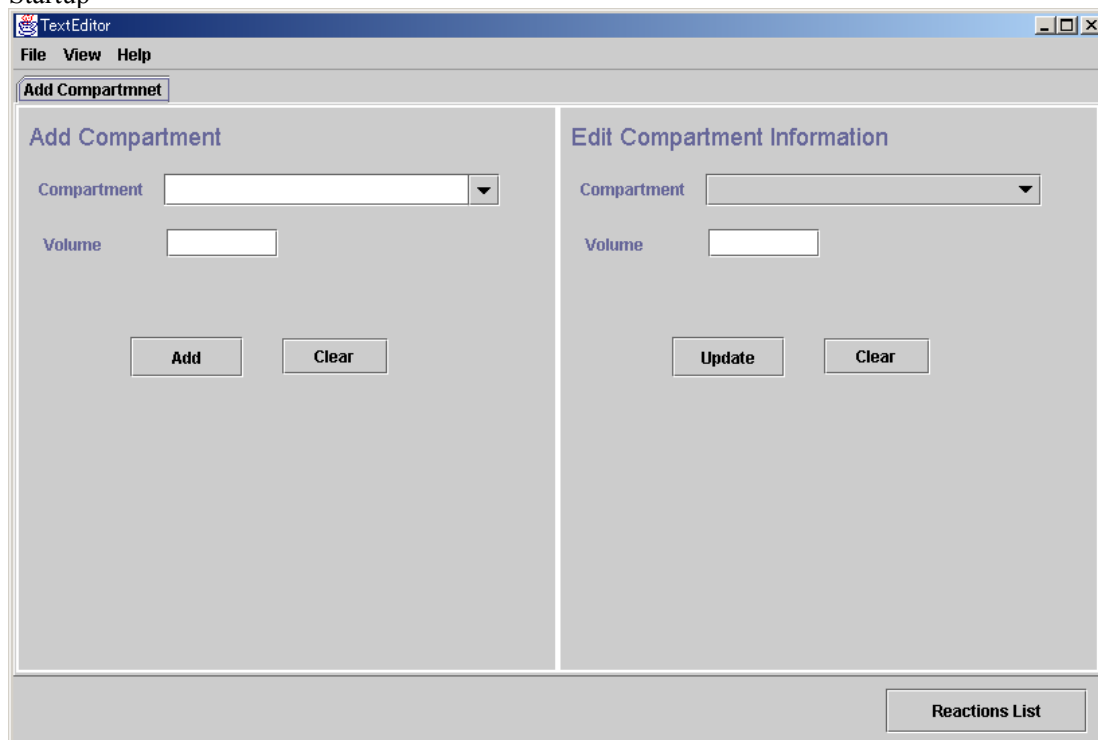
Windows 98, NT4.0, 2000, XP
Java™ 2 Runtime Environment (1.3 is recommended)

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

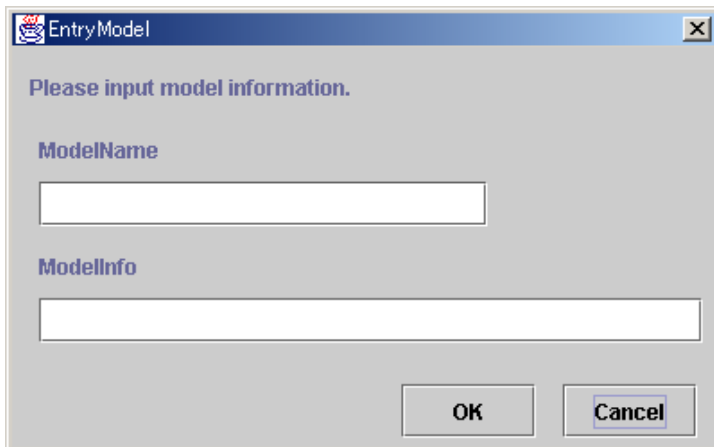
4.1 Model creation

4.1.1 Creation of a new model



Click [File] and select [New].

4.1.2 EntryModel



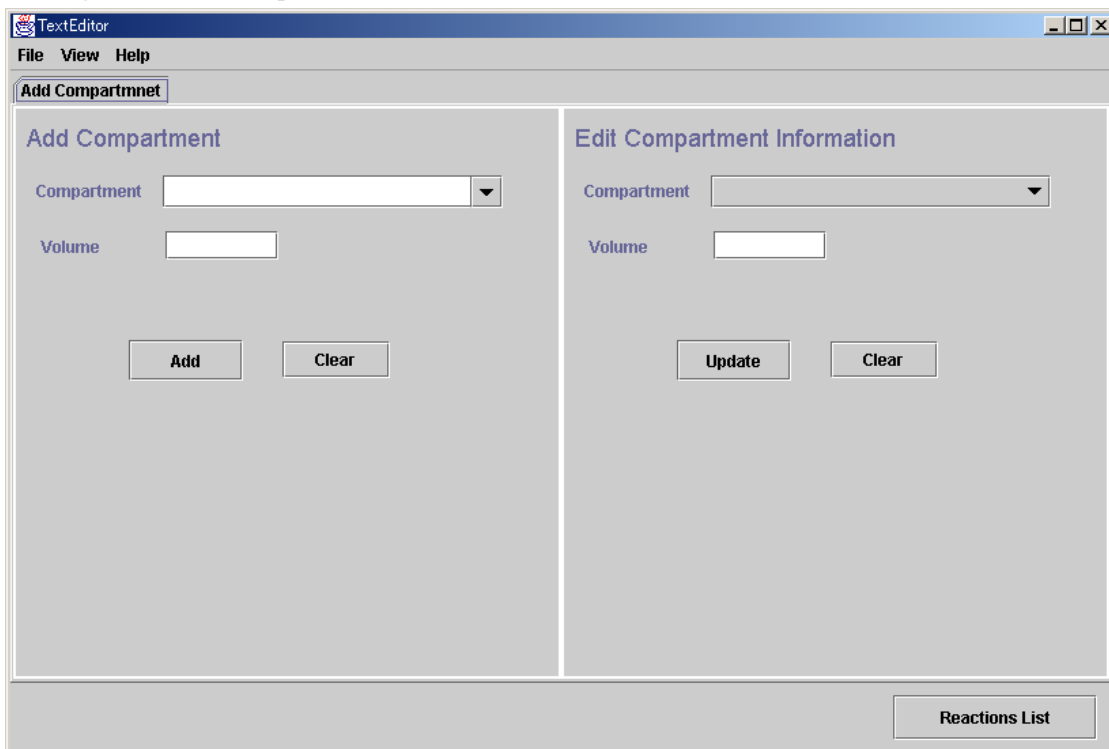
Input "ModelName". If necessary, input "ModelInfo".

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.

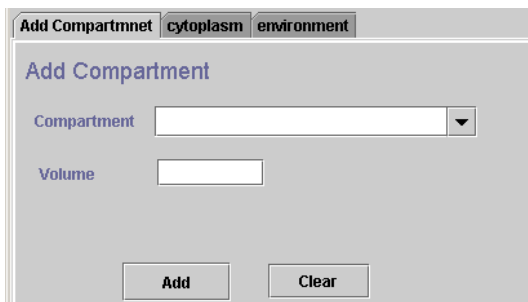
5. Registration of compartment

5.1 Registration of compartment



The screenshot shows a window titled 'TextEditor' with a menu bar containing 'File', 'View', and 'Help'. Below the menu bar is a tab labeled 'Add Compartment'. The main area is divided into two panels. The left panel, titled 'Add Compartment', contains a 'Compartment' dropdown menu and a 'Volume' text input field. Below these are 'Add' and 'Clear' buttons. The right panel, titled 'Edit Compartment Information', contains a 'Compartment' dropdown menu and a 'Volume' text input field. Below these are '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".



The screenshot shows a window with three tabs: 'Add Compartment', 'cytoplasm', and 'environment'. The 'Add Compartment' tab is active. It contains a 'Compartment' dropdown menu and a 'Volume' text input field. Below these are '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

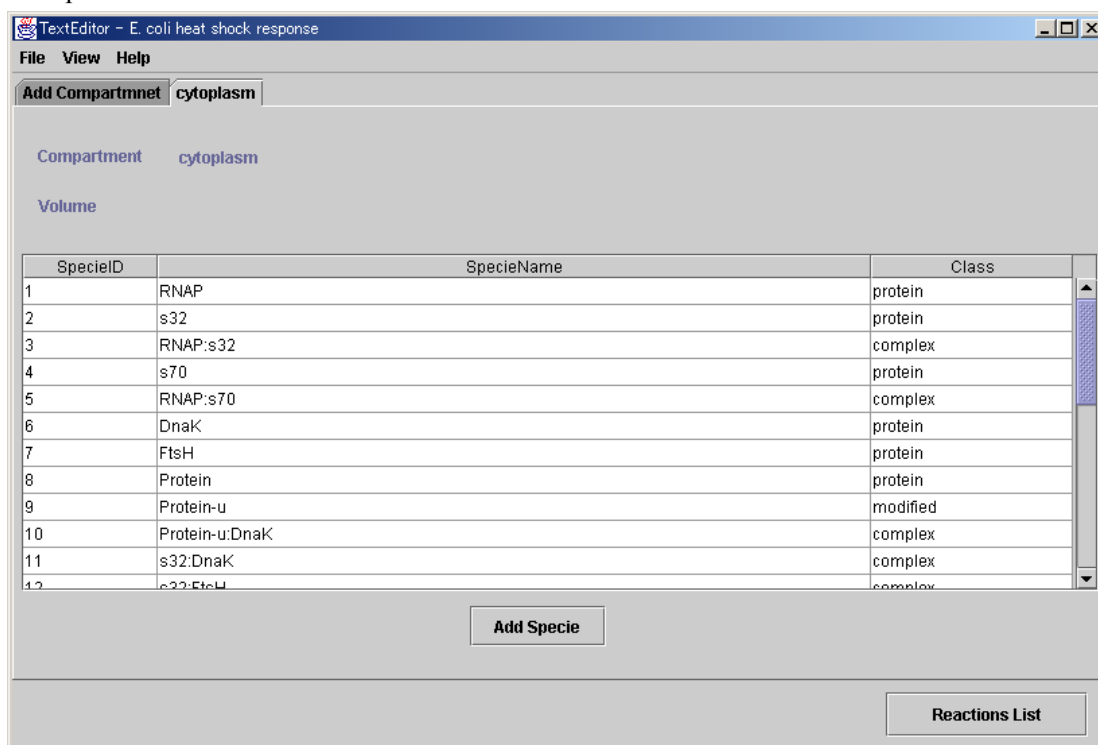
A dialog box titled "Edit Compartment Information" in blue text. It contains two input fields: "Compartment" is a dropdown menu, and "Volume" is a text input field. At the bottom, there are two buttons: "Update" and "Clear".

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.

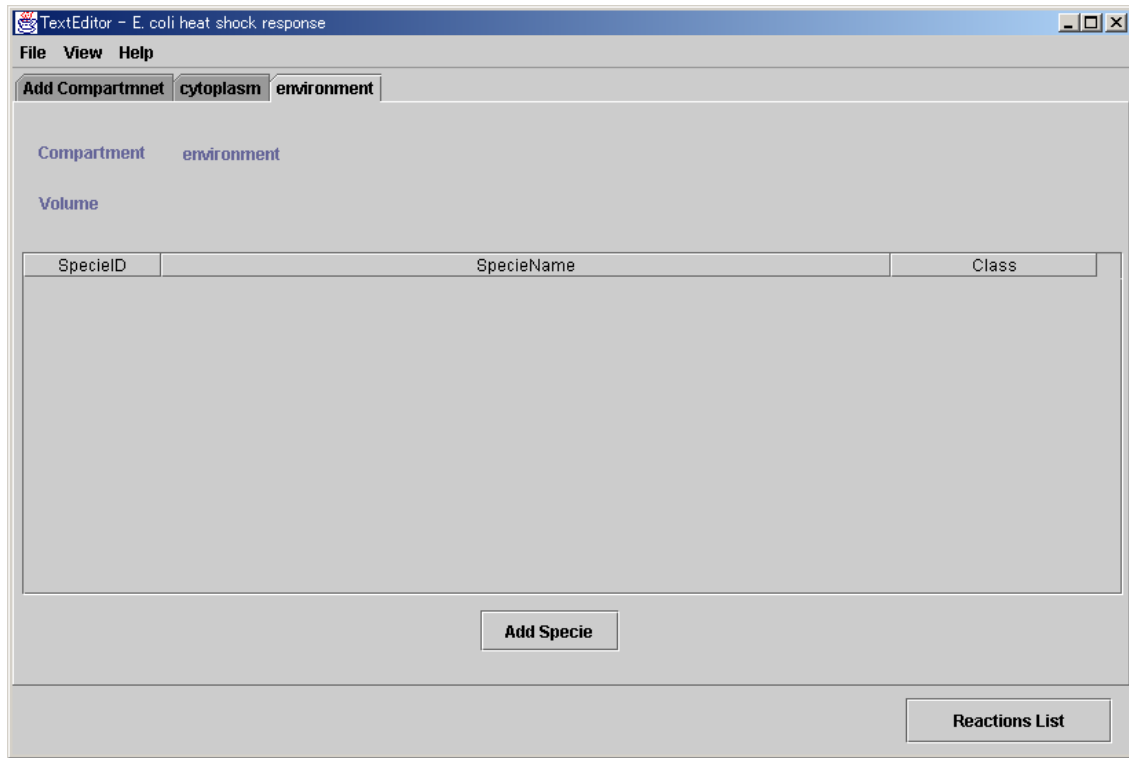
6.1.4 ReactionList button

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



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

The screenshot shows a registration form for a specie. The fields are as follows:

- SpecieID:** 32
- SpecieName:** (empty text box)
- Compartment:** environment (dropdown menu)
- Class:** (empty dropdown menu)
- TotalAmount:** variable (selected), constant (unselected)
- MassBalance:** on (selected), off (unselected)
- Decomposition:** on (selected), off (unselected)
- InitialAmount:** (empty text box)
- List Of Elements:** A table with columns: SpecieName, Compartment, stoichiometry. The table is currently empty.
- Buttons:** 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".

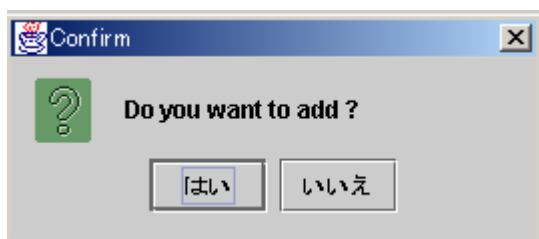
- ListOfElements

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.

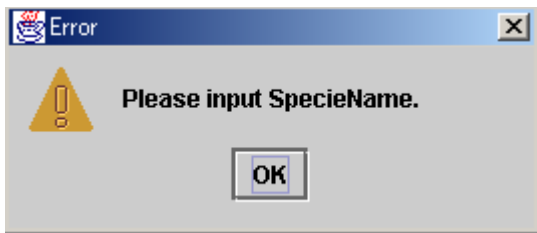
After setting, click the [Add] button to display the confirmation screen. If there is no problem, click [Yes] to register the specie.



Click the [Cancel] button to abandon the registration.

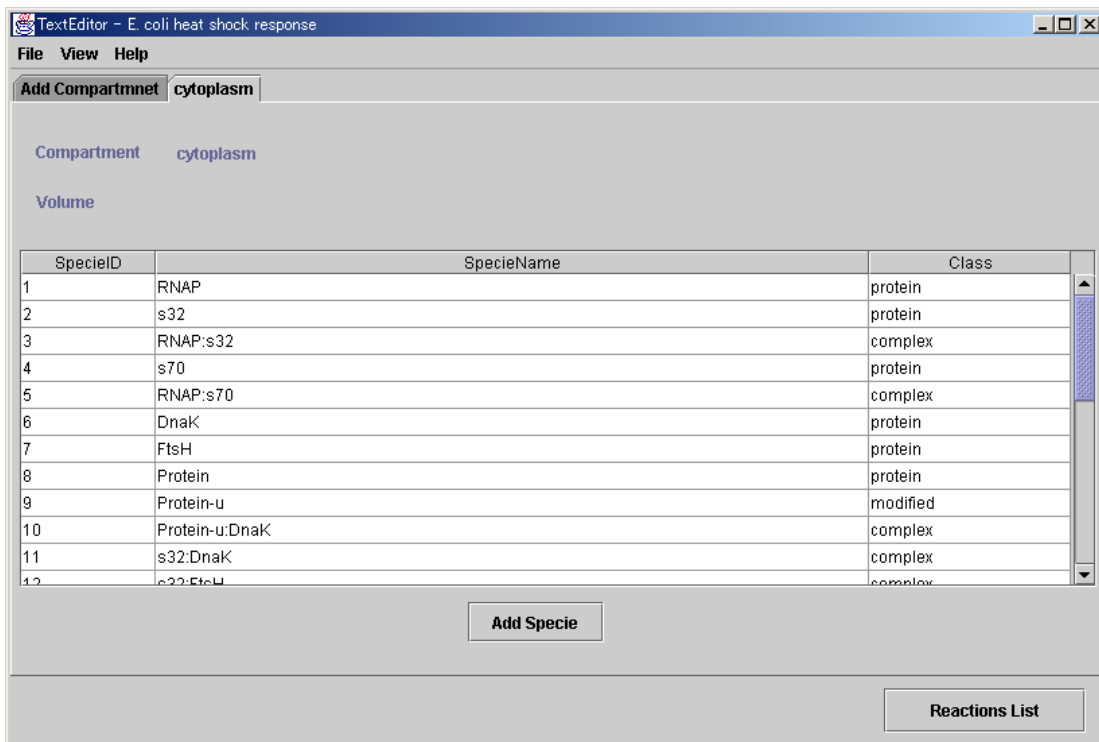
* When the item for input is shortage or required to reedit, the following warning appears.

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



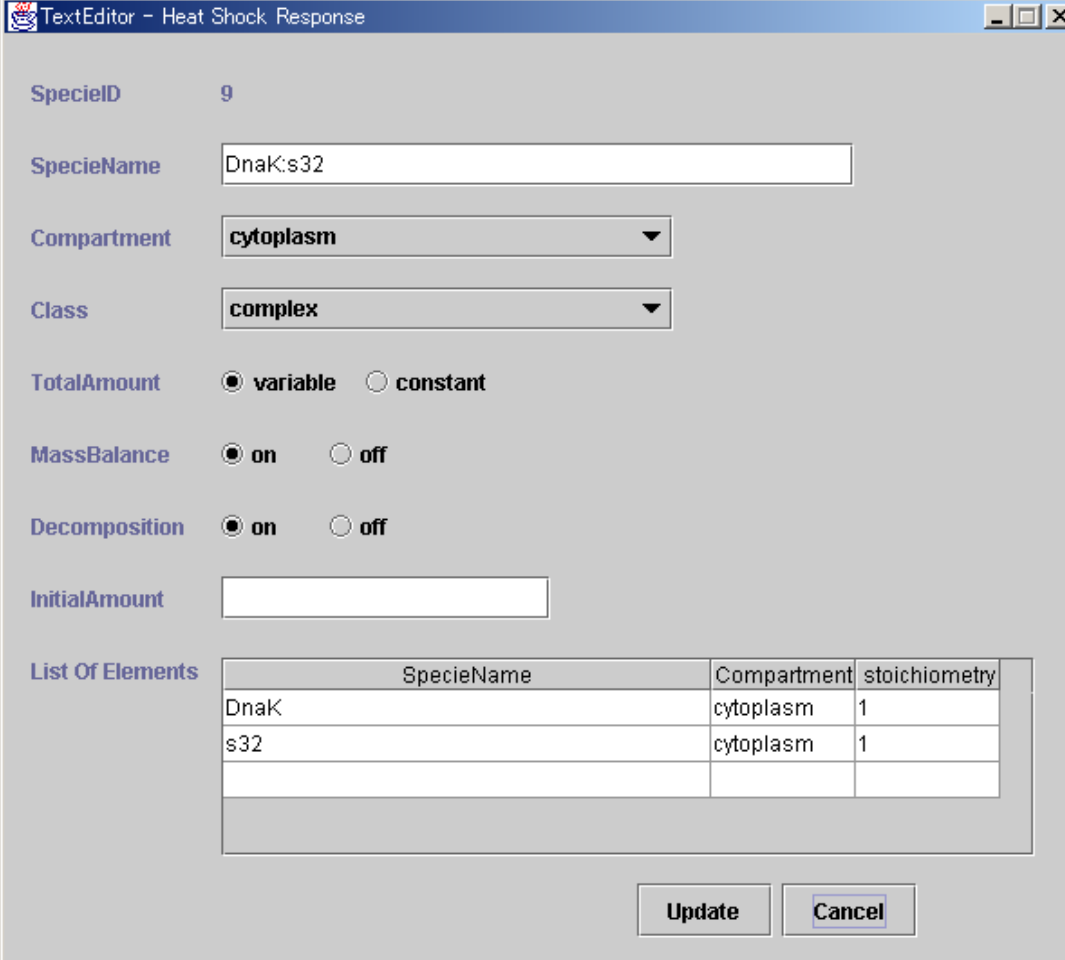
7.2 Species edition

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



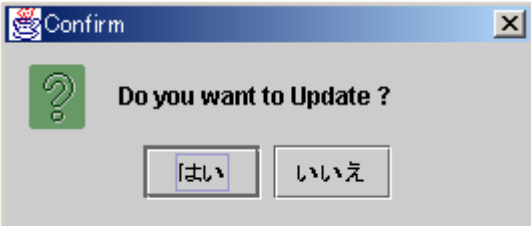
The dialog box 'TextEditor - Heat Shock Response' contains the following fields and options:

- SpecieID**: 9
- SpecieName**: DnaK:s32
- Compartment**: cytoplasm
- Class**: complex
- TotalAmount**: variable constant
- MassBalance**: on off
- Decomposition**: on off
- InitialAmount**: (empty text box)
- List Of Elements**:

SpecieName	Compartment	stoichiometry
DnaK	cytoplasm	1
s32	cytoplasm	1

Buttons: 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.



The 'Confirm' dialog box contains the following elements:

- Icon: Question mark in a green square
- Text: Do you want to Update ?
- Buttons: はい (Yes), いいえ (No)

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.

The screenshot shows a window titled "TextEditor - E. coli heat shock response". The interface includes several fields and controls for configuring a species:

- SpecieID**: 32
- SpecieName**: s32:RNAP:s32
- Compartment**: cytoplasm (dropdown menu)
- Class**: modifier_complex (dropdown menu)
- TotalAmount**: variable constant
- MassBalance**: on off
- Decomposition**: on off
- InitialAmount**: (empty text field)
- List Of Elements**: A table with the following data:

SpecieName	Compartment	stoichiometry
s32	cytoplasm	1

At the bottom of the window are "Update" and "Cancel" buttons.

8. Explanation of screen for listing reactions

8.1 Switching the screen mode for listing reactions



8.1.1 All mode

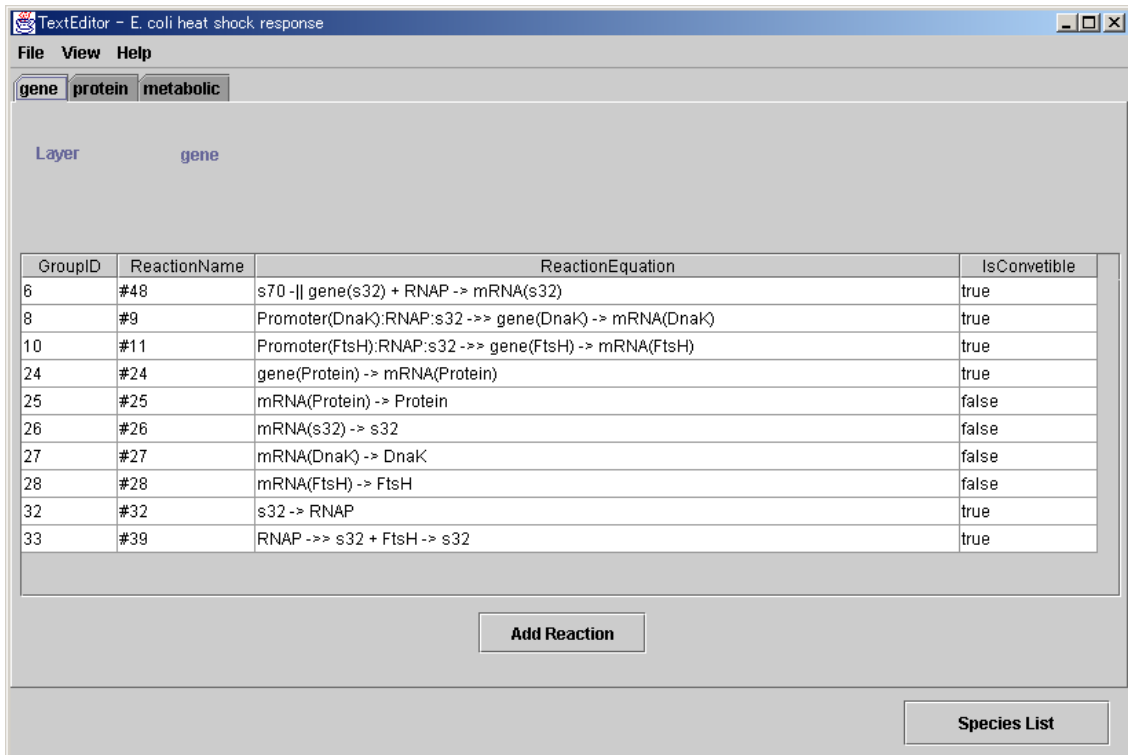
All the reactions are listed despite the value of "isConvertible".

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

A screenshot of a 'TextEditor' window titled 'E. coli heat shock response'. The window has a menu bar with 'File', 'View', and 'Help'. Below the menu bar are three tabs: 'gene', 'protein', and 'metabolic', with 'gene' selected. Underneath the tabs, there are two labels: 'Layer' and 'gene'. The main area contains a spreadsheet with the following data:

GroupID	ReactionName	ReactionEquation	IsConvertible
6	#48	s70 - gene(s32) + RNAP -> mRNA(s32)	true
8	#9	Promoter(DnaK):RNAP:s32 ->> gene(DnaK) -> mRNA(DnaK)	true
10	#11	Promoter(FtsH):RNAP:s32 ->> gene(FtsH) -> mRNA(FtsH)	true
24	#24	gene(Protein) -> mRNA(Protein)	true
25	#25	mRNA(Protein) -> Protein	false
26	#26	mRNA(s32) -> s32	false
27	#27	mRNA(DnaK) -> DnaK	false
28	#28	mRNA(FtsH) -> FtsH	false
32	#32	s32 -> RNAP	true
33	#39	RNAP ->> s32 + FtsH -> s32	true

At the bottom of the window, there are two buttons: 'Add Reaction' and 'Species List'.

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.

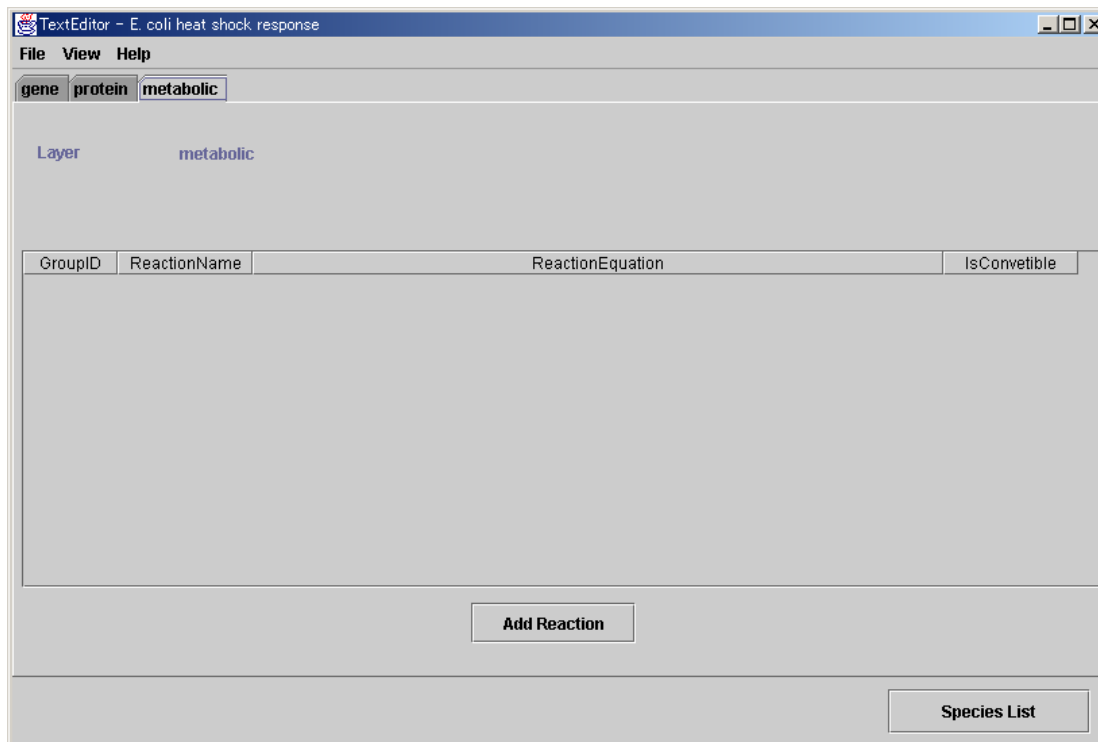
8.2.4 SpecieList button

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



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

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):Acivator ->> 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.

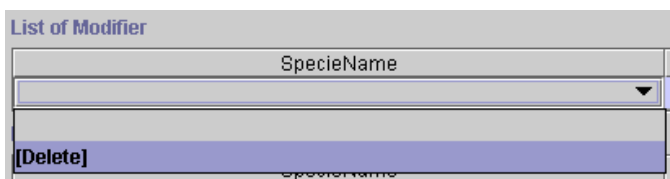
- ReactionEquation

The ReactionEquation is automatically generated. It is ModifierReactionEquation.

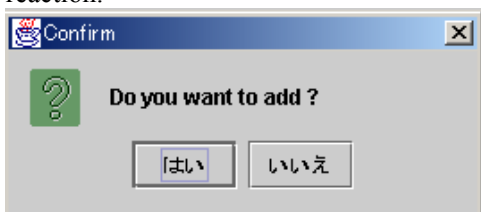
- Stoichiometry

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

Pushing the [Enter] key decides the stoichiometry.

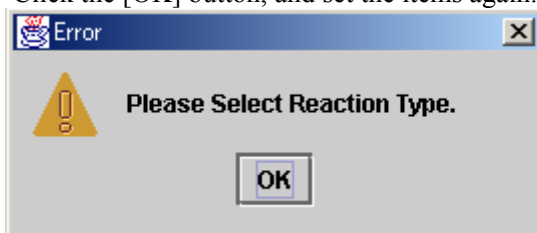


After the setting, click the [Add] button to show the confirmation screen. Clicking [YES] to add the reaction.

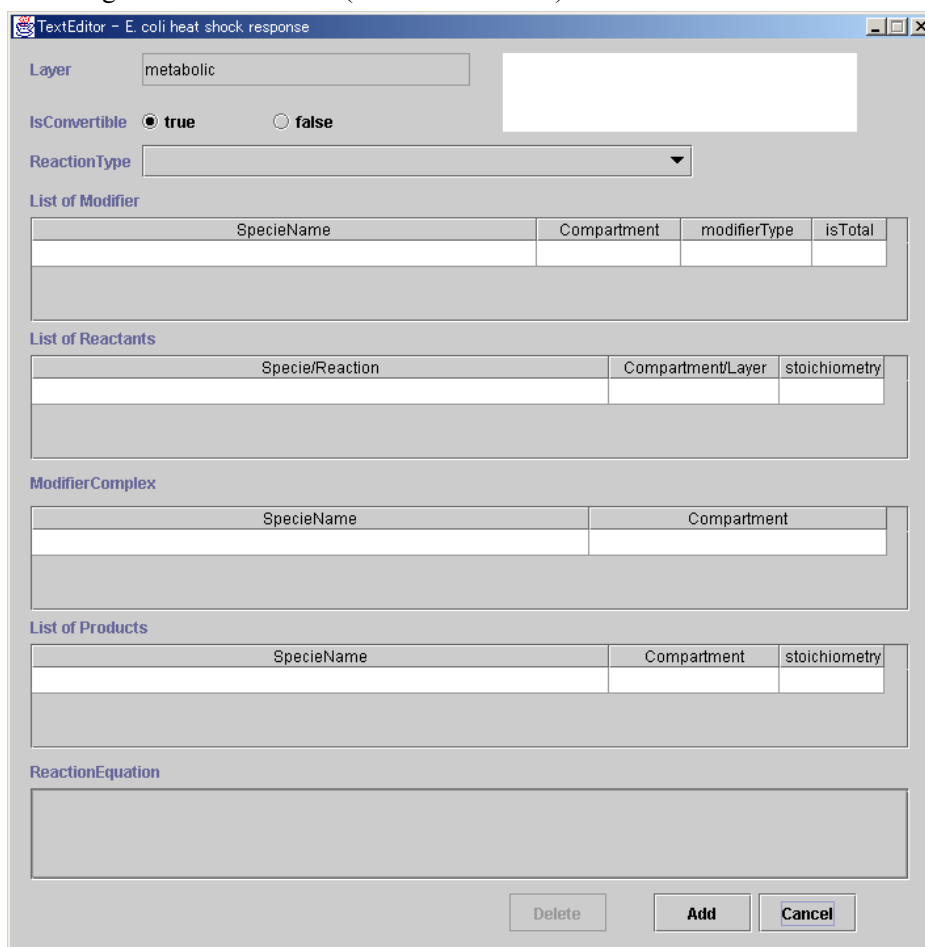


To abandon the registration, click the [Cancel] button.

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



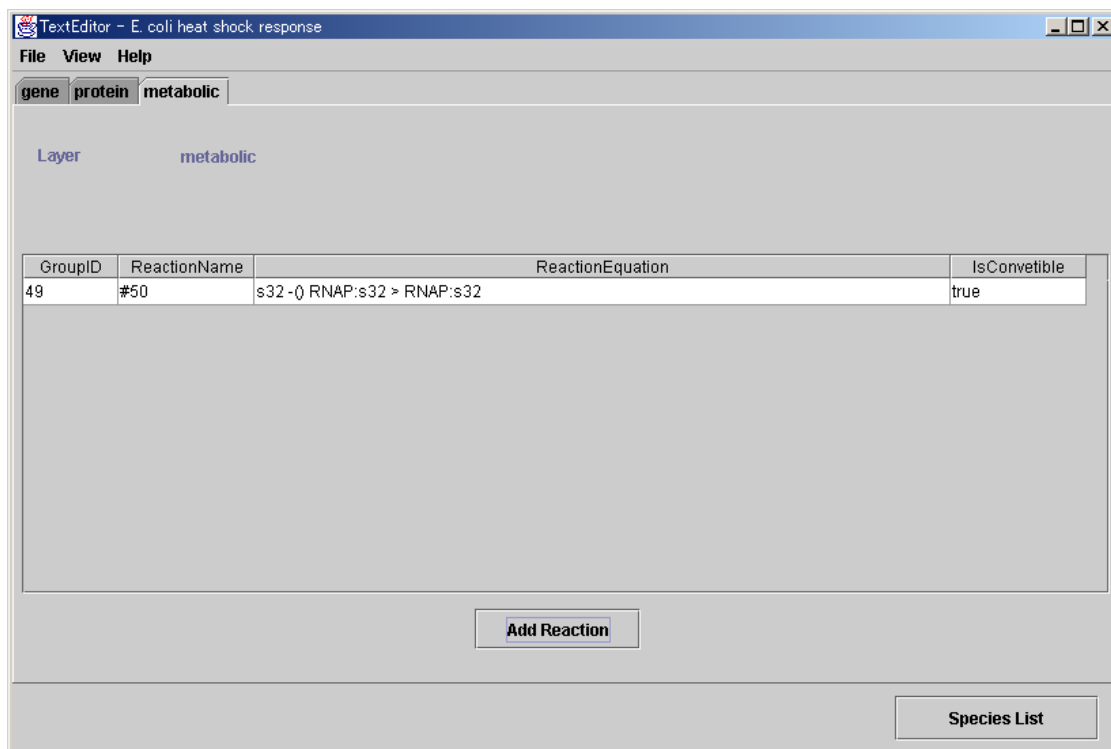
9.1.3 Registration of reaction (Convertible mode)

A screenshot of a software dialog box titled "TextEditor - E. coli heat shock response". The dialog has a light gray background and a blue title bar. It contains several sections: "Layer" with a text field containing "metabolic"; "IsConvertible" with radio buttons for "true" (selected) and "false"; "ReactionType" with a dropdown menu; "List of Modifier" with a table with columns "SpecieName", "Compartment", "modifierType", and "isTotal"; "List of Reactants" with a table with columns "Specie/Reaction", "Compartment/Layer", and "stoichiometry"; "ModifierComplex" with a table with columns "SpecieName" and "Compartment"; "List of Products" with a table with columns "SpecieName", "Compartment", and "stoichiometry"; and "ReactionEquation" with a large text area. At the bottom right, there are three buttons: "Delete", "Add", and "Cancel".

In the “Convertible” mode, multiple 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)

The screenshot shows a window titled "TextEditor - Heat Shock Response" with the following fields and tables:

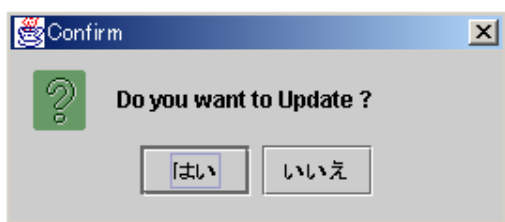
- ReactionID**: 1
- Layer**: protein
- reactionType**: binding
- IsConvertible**: true false
- List of Modifier**: Empty table with columns: SpecieName, Compartment, modifierType, isTotal.
- List of Reactants**:

SpecieName	Compartment	stoichiometry
RNAP	cytoplasm	1
s70	cytoplasm	1
- ModifierComplex**: Empty table with columns: SpecieName, Compartment.
- List of Products**:

SpecieName	Compartment	stoichiometry
RNAP:s70	cytoplasm	1
- ReactionEquation**: RNAP + s70 <-> RNAP:s70

Buttons at the bottom: Delete, Update, Cancel.

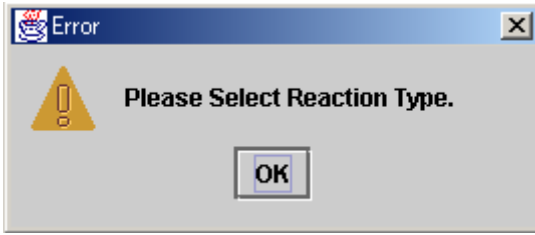
The edition is carried out in the same manner as the registration of the reactions. After setting, click the [Update] button to show the confirmation screen. Click [YES] to update the revision. To reedit, click [NO].



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

Buttons: 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.

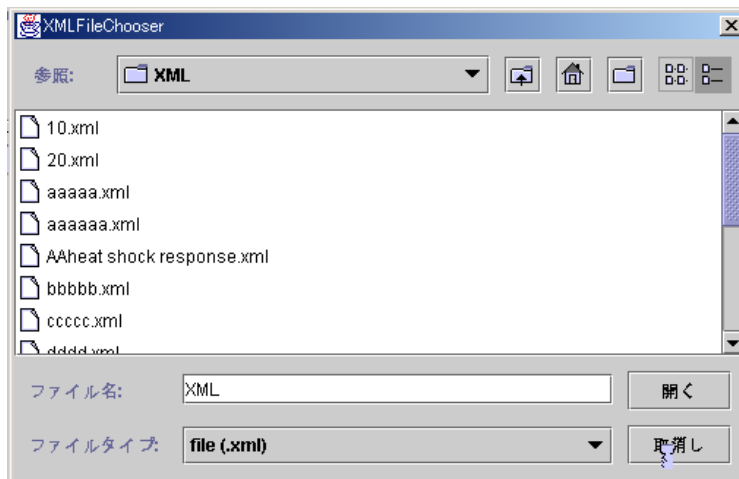
*The reactions with “IsConvertible = false” are omitted from the list on the “Convertible” mode, but the “All” mode displays all the reactions despite the value of “IsConvertible”.

10. Merge Function

10.1 Merge



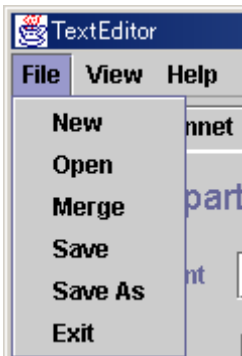
In order to merge the existing network into the current network, choose [Merge] from the "File" menu and select the sanac file to be merged.



* 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

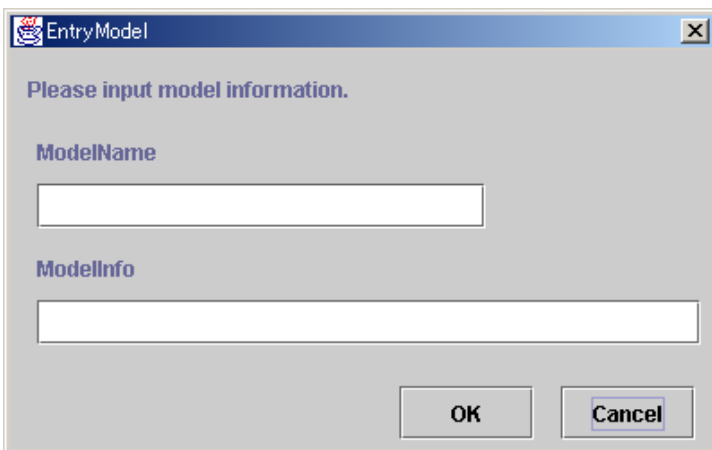
11.1.3 Merge

An existing file is merged into the current file.

11.1.4 Save

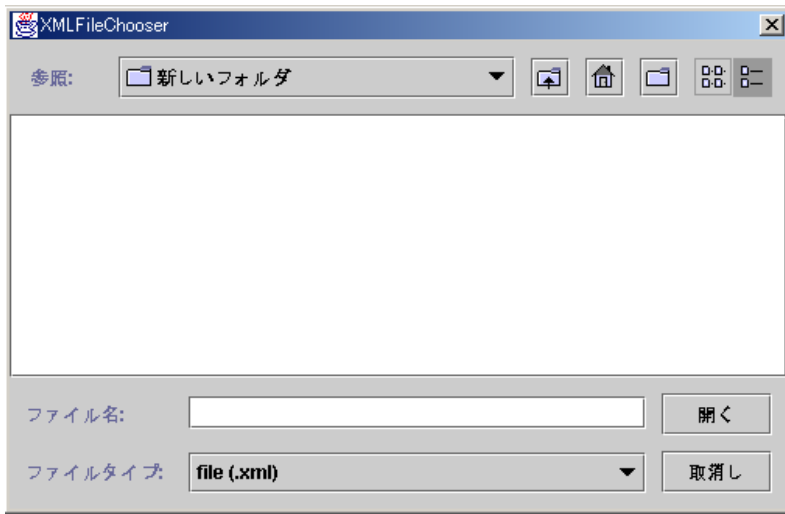
The current network overwrites the existing one, and is saved.

* 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.

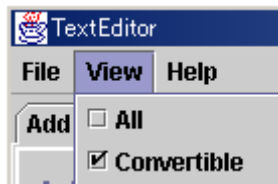


11.1.6 Exit

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.