CADLIVE Ver.2.75
Operation Manual

2007.5. Kyushu Institute of Technology

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1. CADLIVE

CADLIVE is a system for constructing large-scale biological networks (metabolic and gene regulatory networks) using GUI (Graphic User Interface) and saving them as regulator reaction equations in a database in the format compatible to a simulator. It has been developed by Kurata at the Kyushu Institute of Technology together with staffs at Mitsui Knowledge Industry Co., Ltd.

2. System Requirements

Hardware Configuration:

CPU	: Pentium3 1GHz or higher
Memory	: 256MB or more
HDD	: 1 Gb or more recommended

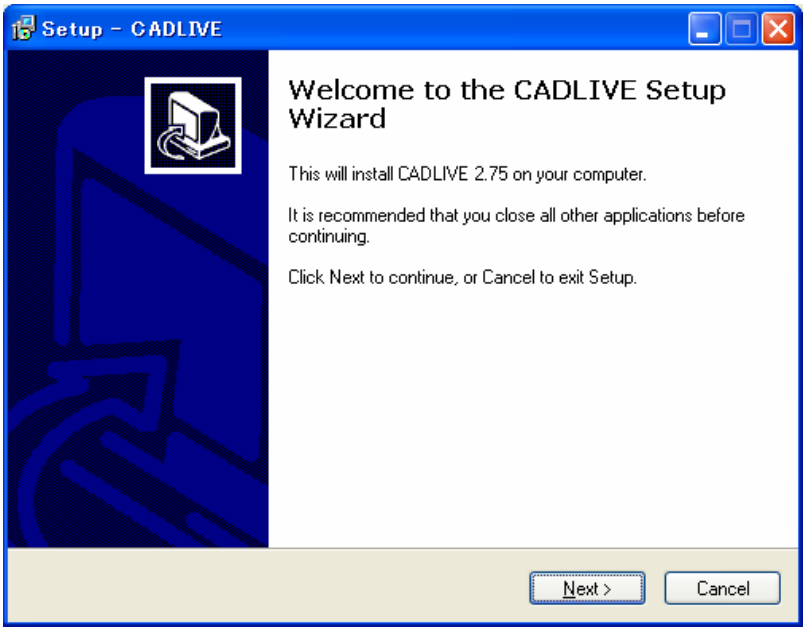
Software Configuration:

Windows 98, NT4.0, 2000, XP
Java™ 2 Runtime Environment 1.3

3. Installation

3-1 Installing CADLIVE

Double-click the “setup.exe” icon on the CD-ROM.
According to the instruction, install CADLIVE in an arbitrary directory.
(Clicking the NEXT button and the Install button installs CADLIVE in the C drive)
At this time, Java™ 2 Runtime Environment is installed simultaneously.



To uninstall CADLIVE, double-click the “unins000.exe” icon installed on the directory. Once CADLIVE is uninstalled, all the existing files as well as the existing network data will be deleted. If you need the network data, make sure to save it as backup on another directory before uninstalling.

4. Start-up

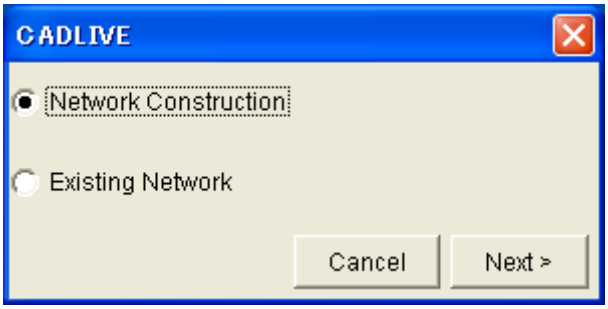
4-1 Start-up of CADLIVE

Make sure that Java™ 2 Runtime Environment (1.3) has been installed. Select CADLIVE from the Program menu or double-click the "CADLIVE32.exe" on the directory (C:¥CADLIVE) where CADLIVE is installed.

Start-up Screen

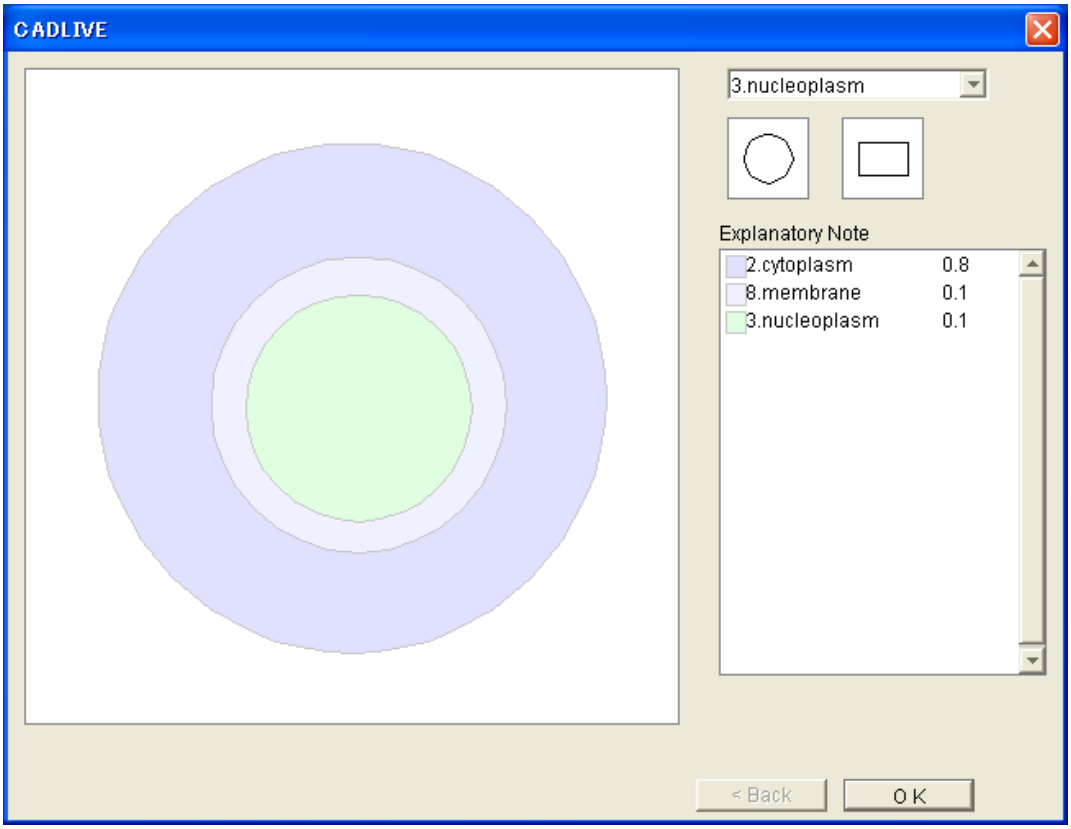
4-2 Creating a New Network

>> OpeningDialog



Select "Network Construction". Click the [Next>] button.

>> Compartment layout using the Cell Comp Dialog box



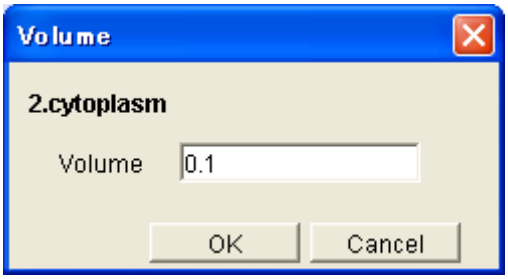
Select Compartments from the select box for editing cellular compartments.

*There are nine types of Compartments: Environment, Cytoplasm, Nucleoplasm, ER, Mitochondria, Golgi, Chloroplast, Membrane and Others.
*If "Others" is selected, its name can be edited arbitrarily.

Select the form (circle or rectangle).
If the panel is clicked, the object will be placed in the designated form of the designated Compartment.

*By dragging the object, it can be moved to a new location.
*By dragging the toggle button on the object, its size can be changed.
*When two objects are overlapped, the overlapping object will have priority over the other. The overlapped part will then be invalid.
* By right-clicking on the object and selecting Delete, the object will be deleted.

>> VolumeDialog



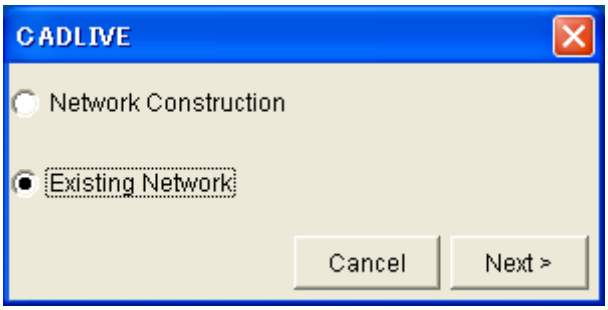
In order to define the Volume of Compartment, select the specified Compartment and click the Volume on the right-click menu. Put an appropriate value in the Volume box and click the [OK] Button.

* Regarding Compartment whose name is the same, setting the value of Volume reflects all the values of Compartment Volume.

After finishing placing all objects, click the [OK] button.

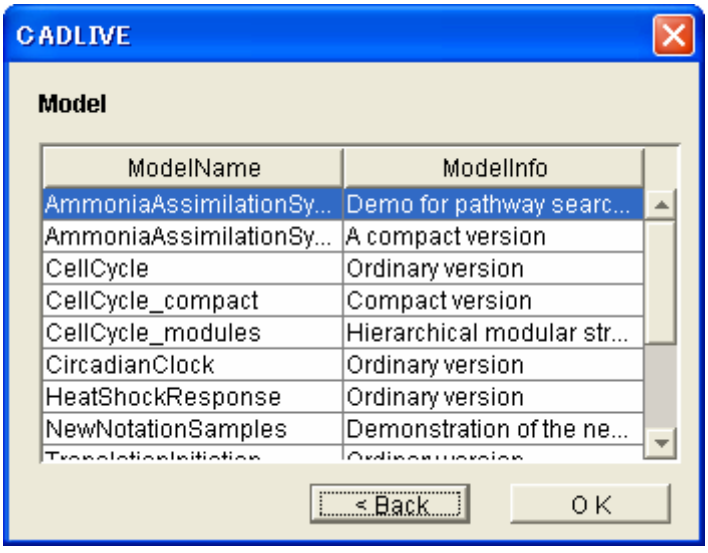
4-3 Loading existing Network

>> OpeningDialog



Select the Existing Network.
Click the [Next>] button.

>> OpenNetWorkDialog

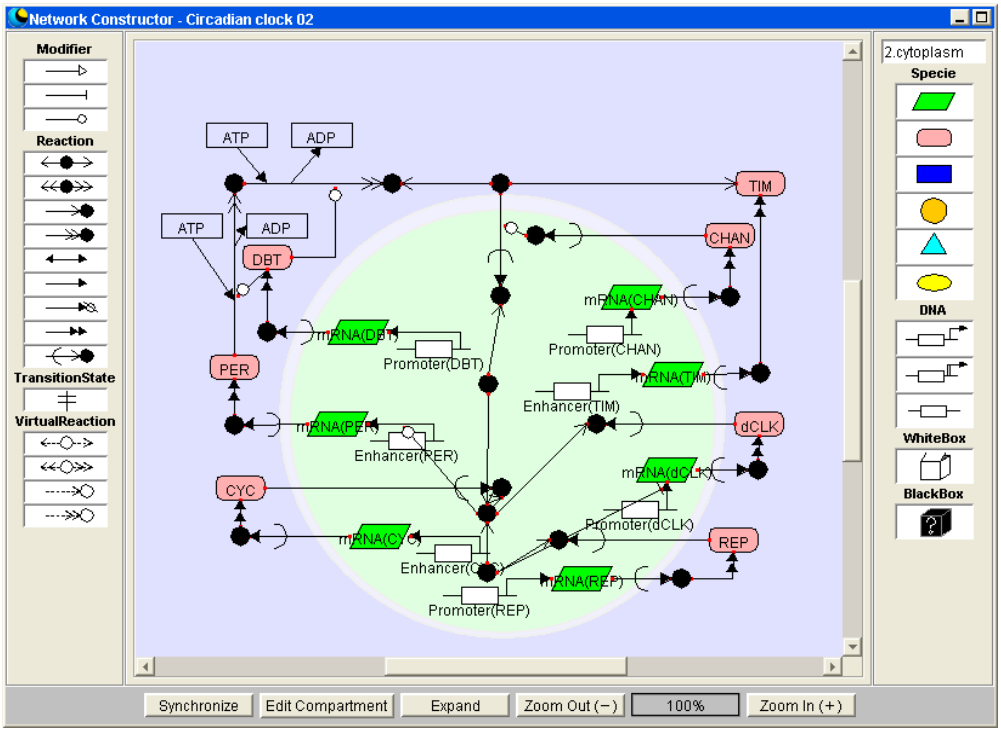


"ModelName" and "ModelInfo" will be displayed in a list. Select the ModelName of the network to load. Click the OK button.

*The CADLIVE GUI Editor is not allowed to import the data that are created and edited by TextEditor.

5. Network Constructor

5-1 Explanation of Objects on the Network Constructor



5-1-1 Panel

This is the field used to position and draw Symbols. One sees the Compartments that have been selected from the Compartment Dialog box.

5-1-2 Modifier Palette

This palette is used to position activator, inhibitor, or enzyme.

5-1-3 Reaction Palette

This palette is used to position binding, binding_with_stoichiometric_changes, homo_association_or_modification, homo_association_or_modification_with_stoichiometric_changes, reversible_conversion, irreversible_conversion, transitionState, degradation, transport, or translation.

5-1-4 Virtual Reaction Palette

This palette is used to position virtual_binding, virtual_binding_with_stoichiometric_changes, virtual_homo_association_or_modification, virtual_homo_association_or_modification_with_stoichiometric_changes.

5-1-5 Species Palette

This palette is used to position RNA, protein, metabolite, environmental_factor, ion_sygnal, others, whitebox, blackbox.

5-1-6 Gene Palette

This palette is used to position transcription, protein_synthesis, or regulatory regions of a gene (enhancer, promoter, other).

5-1-7 WhiteBox Palette

This palette is used to position WhiteBox.

5-1-8 BlackBox Palette

This palette is used to position BlackBox.

5-1-9 Compartment Display Box

This box displays the Compartment that is selected in the panel.

5-1-10 Equation Display Box

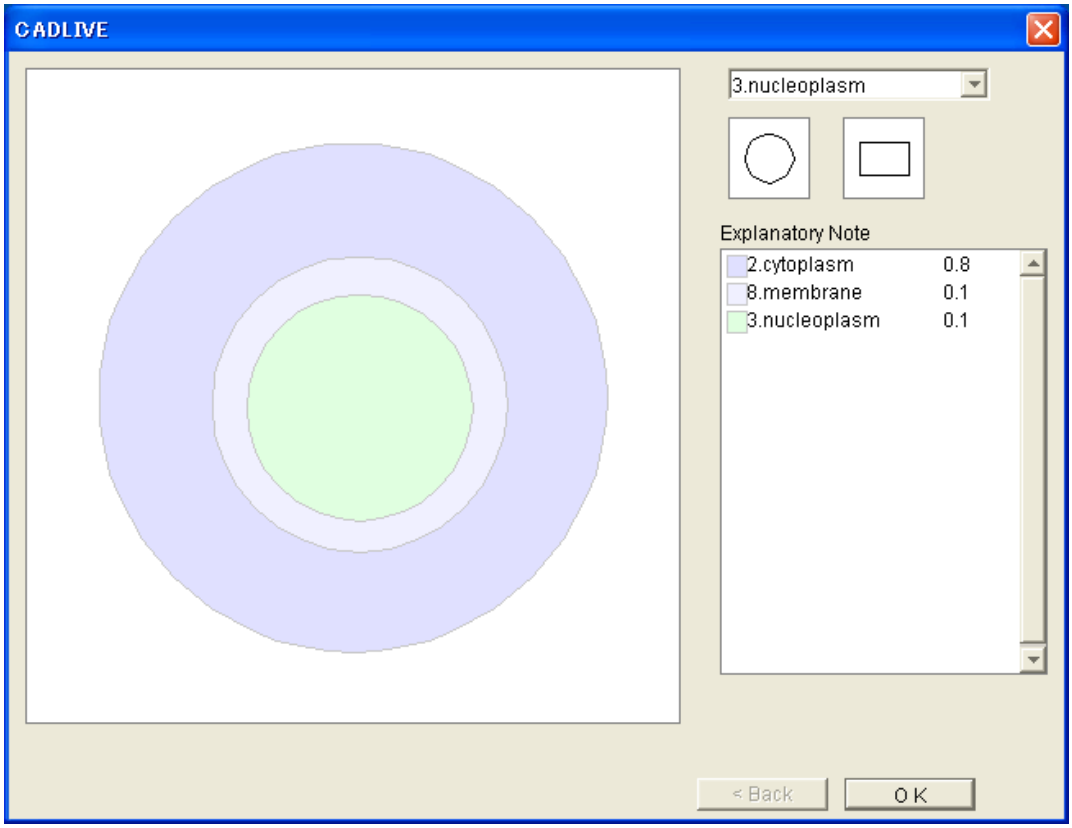
This box displays the Modifier Reaction Equation selected on the panel.
Clicking the Modifier displays the Modifier Reaction Equation, when the modifier is connected to the reaction.

5-1-11 Synchronize Button

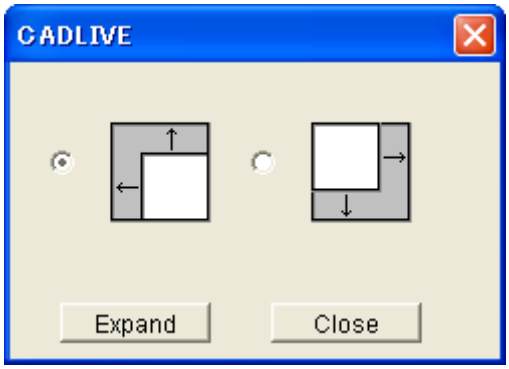
Clicking this button will synchronize data on the Network Constructor with the other Windows.

5-1-12 Edit Compartment Button

Clicking this button will display the Window to reedit Compartments.

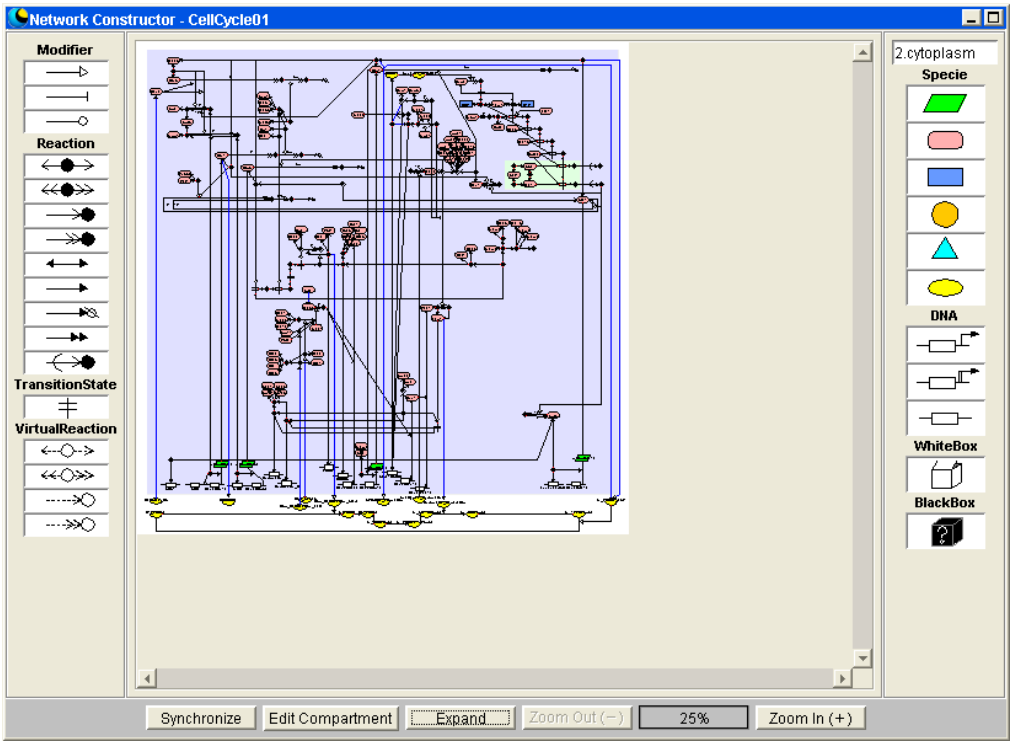


5-1-13 Expand Button



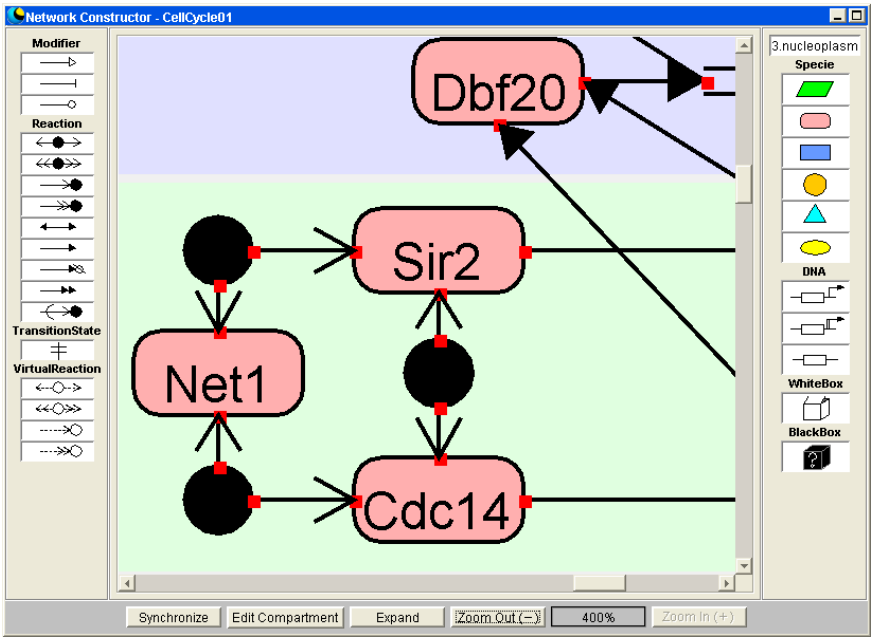
Clicking this button will expand the drawing area of the panel in the upper left or lower right direction. Since the area of the environment is enlarged, one can change the size of the area of cellular compartments of interest.

5-1-14 Zoom Out Button



Clicking this button will reduce the viewing area of the panel (Individual Symbols will be reduced accordingly). The area can be zoomed out up to 25%.

5-1-15 Zoom In Button



Clicking this button will expand the viewing area of the panel (Individual Symbols will be enlarged accordingly). The area can be zoomed in up to 400%.

5-1-16 Zoom Magnification Display Box

The box displays the current zoom magnification.

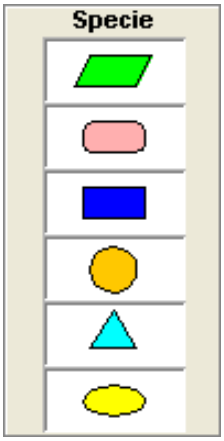
5-2 Positioning Symbols

5-2-1 Positioning Species

The Species is an element that expresses a molecule and can become a node of biological networks.

>> Positioning Species

Click any Species to be positioned on the Species palette, making it "selected."
Click the Species once again at the location that you want to position it in the panel. The Species will be positioned in the panel.
The Species data that is set in the spreadsheet of the Data Editor is displayed at the same time as the Species is placed on the panel.



"RNA"	denotes RNA.
"protein"	denotes Protein.
"metabolite"	denotes Metabolite.
"environmental_factor"	denotes Environmental Factor.
"ion_signal"	denotes Ion Signal.
"others "	denotes Others.
"DNA "	denotes DNA.

* Use Gene (5-2-4) for layout.

"Complex" denotes a complex.
* Position a complex using binding, homo_association_or_modification (5-2-2).

"Modified" denotes a modified substance.
* Position a modified substance, use binding_with_stoichiometric_changes, homo_association_or_modification_with_stoichiometric_changes (5-2-2).

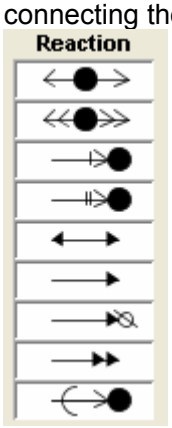
"text_option" denotes text data necessary for detailed reactions.
* Position text_option using Option of Reaction (5-2-8).

"small_molecule_option" denotes a small compound.
* Position small_molecule_option using Option of Reaction (5-2-8).

5-2-2 Positioning Reaction

Reactions are the elements that are described as lines of biochemical networks, denoting various biochemical reactions and formations of complexes.

>> Positioning Reaction
Click any Reaction to be positioned on the Reaction palette, making it "selected." Click the Reaction one more time at the location where you want to position it on the panel. The reaction is placed on the panel. By dragging either node of the reaction onto the Symbol of the Species, reaction can be connected with the species. The end of the arrows turns red in color when the species is successfully connected to the reaction. The reaction data appear in the spreadsheet of the Data Editor in the timing of connecting the reaction arrow to the Species that satisfies the reaction equation.



"binding" denotes the reaction that forms a complex.

"binding_with_stoichiometric_changes" denotes the reaction that forms a complex with a chemical process (stoichiometric changes).

"homo_association_or_modification" denotes the association of identical molecules.

"homo_ association_or_modification_with_stoichiometric_changes" denotes the modification of small molecules.

"reversible_conversion" denotes reversible conversion.

"irreversible_conversion" denotes irreversible conversion.

"degradation" denotes degradation reaction.

"translation" denotes translation reaction.

"transport" denotes transport reaction.
* If transport is used, a Species identical to its reactant will automatically be registered in the Compartment where the species is transported.

"elimination" denotes eliminating a molecule from the complex.

"elimination_with_stoichiometric_changes"
denotes eliminating a molecule from the modified molecule.
* Use Option (5-2-7) for elimination and elimination_with_stoichiometric_changes.

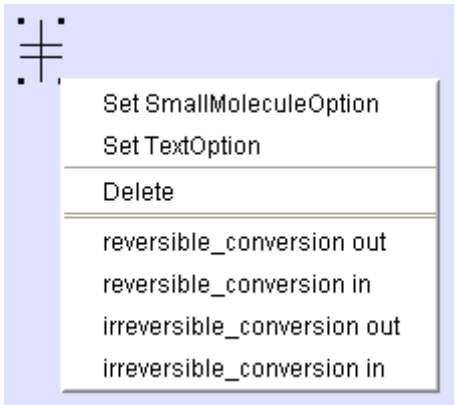
"reversible_conversion_regarding_multicompornent"
denotes reversible conversion regarding multiple species.

"irreversible_conversion_regarding_multicompornent"
denotes irreversible conversion regarding multiple species.
*Position reversible_conversion_regarding_multicompornent and irreversible_conversion_regarding_multicompornent using the Symbol of TransitionState.
* Position unknownReaction using the BlackBox

Select "Set Binding" from the right-click menu to create a complex that consists of more than three components using "binding" or "binding_with_stoichiometric_changes".

Click the “TransitionState” on the Reaction palette, making it "selected".

Click it once again at the location that you want to position it in the panel.
Transition State will be positioned in the panel.



If TransitionState is right-clicked, Set SmallMoleculeOption, Set TextOption, Delete, reversible-conversion out, reversible-conversion in, irreversible-conversion out, irreversible-conversion in will be displayed.
Thus, when creating reversible_conversion_regarding_multicompornent, use reversible-conversion out and reversible-conversion in,

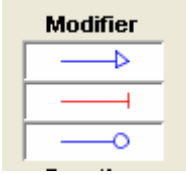
and when creating irreversible_conversion_regarding_multicompornent,
use irreversible-conversion out and irreversible-conversion in.

“transcription”
”protein_synthesis”
* Position transcription and protein_synthesis using Gene (5-2-4).

5-2-3 Positioning Modifier

The Modifier is an enzyme that catalyzes reaction, or a regulator that activates or inhibits a reaction. Regulators can also express the reaction for activation or inhibition of the Species or another Modifier.

>> Positioning a Modifier
Click Modifier on the Modifier palette, making it "selected."
Click it once again at the location that you want to position it in the panel.
Modifier will be positioned in the panel.



"activation" denotes Activation.

"inhibition" denotes Inhibition.

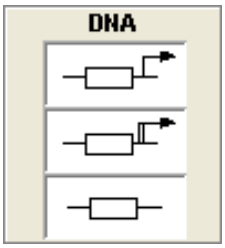
"enzyme" denotes Enzyme Reaction.

* Enzyme can be connected only to protein, complex, and modified
* Position unknownModifier using the BlackBox

5-2-4 Positioning Gene

Functions of Gene are Species elements such as DNA and transcription, as well as reaction elements such as protein synthesis.

>> Positioning Gene
Click Gene on the DNA palette, making it "selected."
Click it once again at the location that you want to position it in the panel.
Gene will be positioned in the panel.



"transcription" collectively denotes the coding region and transcription reaction.
"protein_synthesis" collectively denotes the coding region, transcription and translation reaction.
"other_gene" denotes regulatory regions (enhancer or promoter).

* Transcription is connected only to RNA.
* "protein_synthesis" is connected only to protein. When using protein_synthesis, RNA will be registered as a Species while transcription and translation will be registered as Reactions.

5-2-5 Positioning WhiteBox

WhiteBox denotes the subnetwork whose details are known (or predicted) clearly.
It can collect the subnetwork into one symbol by registering specific symbols on a panel to WhiteBox.
Creating WhiteBox does not have any influence on the equation of the existing networks.

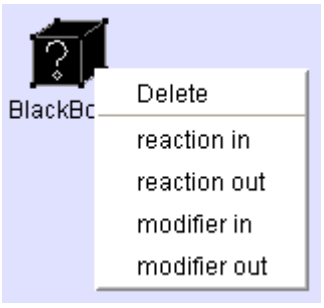
>> Positioning WhiteBox
Click the symbol to store in WhiteBox on the panel, making it "selected."
When selecting the complex symbols, pressing the Ctrl key and click them.
By clicking the WhiteBox in the state where the symbol to store was selected, WhiteBox is positioned on the Panel.
Expanding/storing operation after location is run on WhiteBoxTreeWindow. (7 chapters of reference)

*It is allowed to store the WhiteBox in other WhiteBox.
*It is not allowed to store the symbols that stored in WhiteBox in other WhiteBox.
*To delete the symbols stored in WhiteBox, WhiteBox needs to be deleted.
*By storing the symbols that become Reactant of Degradation in WhiteBox, the Reactant of Degradation is also stored.
*By storing the Species by which Domain division in Whitebox, all divided Domain is stored in WhiteBox.

5-2-6 Positioning BlackBox

"BlackBox" denotes a subnetwork whose molecular mechanism are unknown.
It is allowed to place an unknown subnetwork as a BlackBox symbol.

>> Positioning BlackBox
Click the BlackBox on the palette, making it "selected."
Click the BlackBox one more time at the location where you want to position it on the panel.
The BlackBox is placed on the panel.



>> Positioning unknown reaction
By right-clicking on the BlackBox on the blackbox panel and selecting "reaction in" or

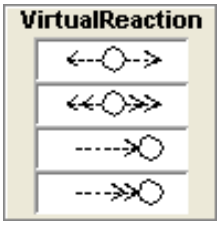
"reaction out", an unknown reaction is placed on the panel.

>> Positioning unknownModifier
By right-clicking on the BlackBox on the panel and selecting "modifier in" or "modifier out", an unknown modifier is placed on the panel.

* BlackBox is treated in the same manner as a single Species on the data editor.

5-2-7 Positioning VirtualReaction

"VirtualReaction" is the reaction that does not occur in fact. It is an element for specifying reaction sites or the sequences of complicated reactions.
VirtualReaction is always attached to "VirtualNode".

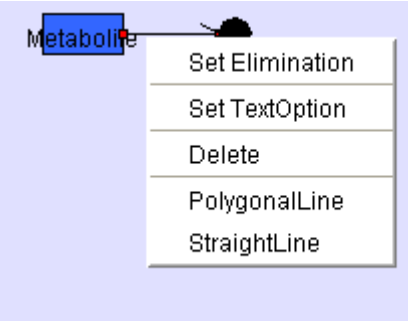


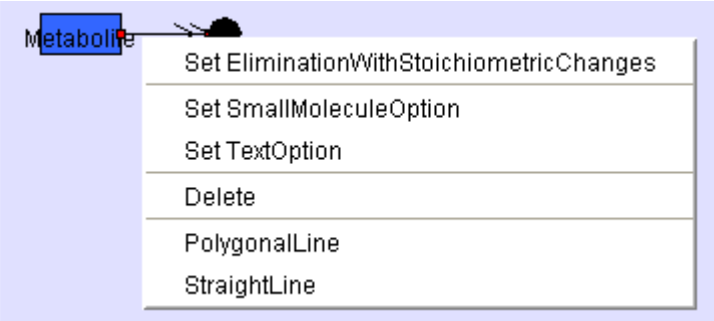
>> Positioning VirtualReaction
Click the VirtualReaction on the VirtualReaction palette, making it "selected."
Click the VirtualReaction one more time at the location where you want to position it on the panel, it will be placed on the panel.
The VirtualReaction data appear in the spreadsheet of the FrameworkEditor when connecting the VirtualReaction arrow to Species, VirtualNodes, or Domains that satisfy the reaction equation.

5-2-8 Positioning Option

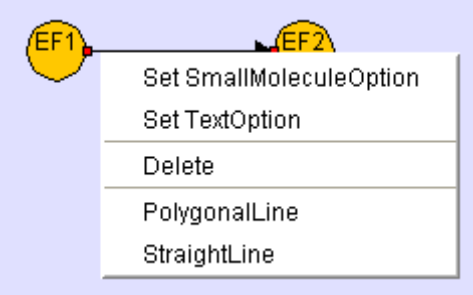
>> Positioning elimination, elimination _with_stoichiometric_changes, virtual_elimination, virtual_ elimination _with_stoichiometric_changes

Right-click homo_association_or_modification, homo_association_or_modification_with_stoichiometric_changes, virtual_ homo_association_or_modification, virtual_homo_ association_or_modification_with_stoichiometric_changes, and select SetElimination or SetEliminationWithStoichiometicChanges



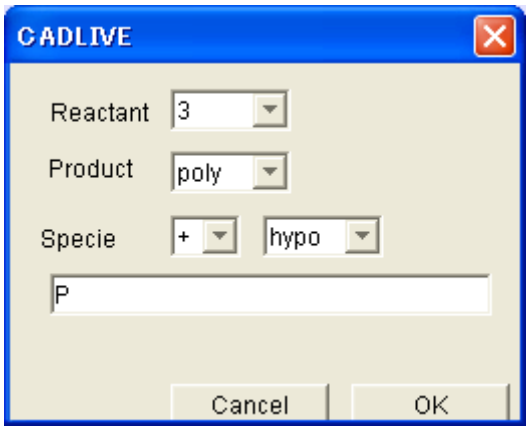


>> Positioning Text Option



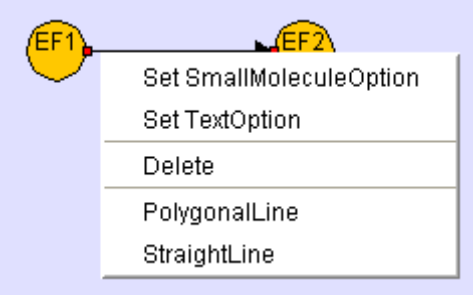
Right-click Reaction or VirtualReaction that is allowed to use Text Option, (binding, binding_with_stoichiometric_changes, homo_association_or_modification, homo_association_or_modification_with_stoichiometric_changes、elimination, elimination_with_stoichiometric_changes、reversible_conversion, irreversible_conversion_reversible_conversion_regarding_multi_component, irreversible_conversion_regarding_multi_component, virtual_homo_association_or_modifiation, virtual_homo_association_or_modification_with_stoichiometric_changes, virtual_elimination、virtual_elimination_with_stoichiometric_changes) to open TextOption and select SetTextOption.

Input option data in the following TextOptionDialog box.



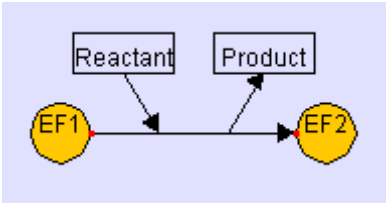
* Input the number of Species on the Reactant side of Reaction to which Text Option will be added (can be selected from numbers from 2 to 10, or Poly, Hyper or Hypo).
* Input the number of Species on the Product side of Reaction to which Text Option will be added (can be selected from numbers from 2 to 10, or Poly, Hyper or Hypo).
* Input the Species data to which Text Option will be added.
If the data is "+," it will be registered in Reactant.
If it is "-," it will be registered in Product.
However, it will be always positive in homo_association_or_modification or homo_association_or_modification and it will be always negative in elimination, elimination_with_stoichiometric_changes.
* The number of TextOptionSpecie can be selected from numbers between 2 and 10, or Poly, Hyper or Hypo.
The name input in the lower box will be registered as Species Name or VirtualNodeName.

>> Layout of Small Molecule Option

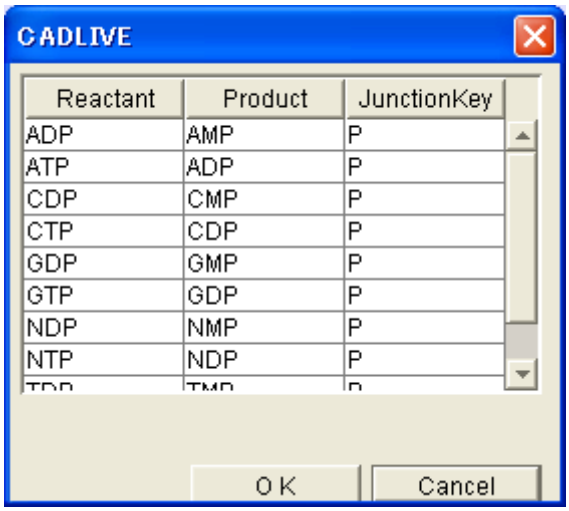


Right-click Reaction that is allowed to use Small Molecule Option, and select SetSmallMoleculeOption.

In order to add Option to ReversibleConversion, IrreversibleConversion, reversible_conversion_regarding_multi_component, or irreversible_conversion_regarding_multi_component, the name of reactants and products can be edited. The default for Reactant and Product is as follows.



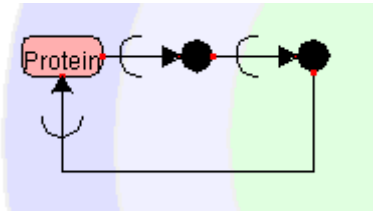
To set SmallMoleculeOption regarding homo_association_or_modification_with_stoichiometric_changes, virtual_homo_association_or_modification_with_stoichiometric_changes, elimination_with_stoichiometric_changes, or virtual_elimination_with_stoichiometric_changes, select Reactant and Product from the dialog box.



The substance in JunctionKey will be added to Modified.
VirtualReaction is ignored.

>> Positioning Option Transport

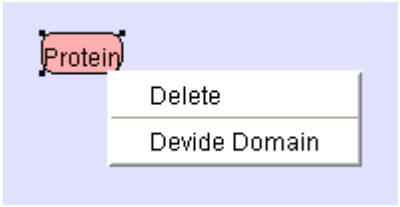
By right-clicking on the transport and selecting "SetOptionTransport", users are able to draw the reversed transport.

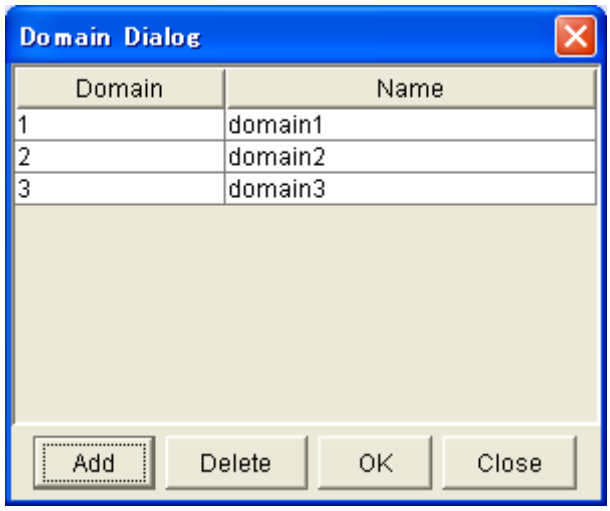


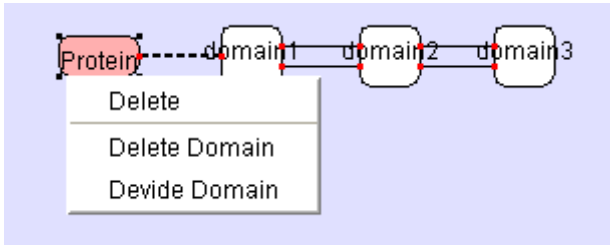
Since "Option transport" is able to connect not only to the transported Reactant but also to the related Species, users are able to draw the transportation between multiple compartments.

5-2-9 Positioning Domain

Domain denotes the binding sites or functional sites of RNA or Protein.
Each Domain can be named and linked to VirtualReaction.







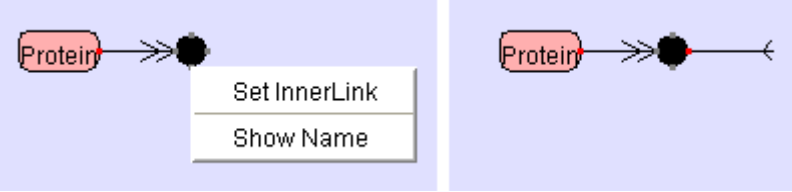
Select "Divide Domain" from the right-click menu of RNA or Protein to divide, displaying Domain Dialog.

Click the Add Button to add a new Domain.
Specifying the name of Domain and clicking the OK button display the Domain on NetworkConstructor.
When deleting a specific Domain, select the specific domain to delete and click the Delete button.

When editing the created Domain, select "Divide Domain". DomainDialog will be opened and can be edited.

5-2-10 Positioning InnerLink

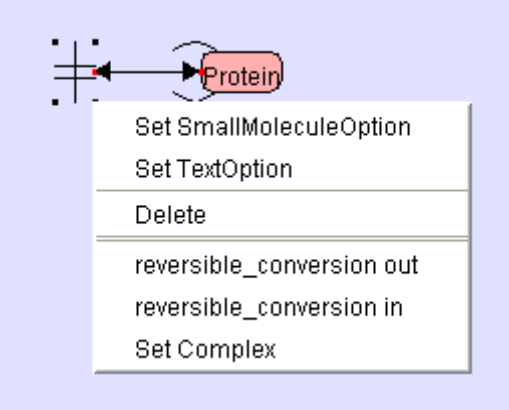
InnerLink connects Species to Virtual Nodes, which makes clear how virtual nodes and real nodes constitute the Species.



By selecting "Set InnerLink" from the right-click menu of "complex" or "modified" that is an origin of link, InnerLink will be displayed on NetworkConstructor.

5-2-11 Positioning ExchangeComplexReaction

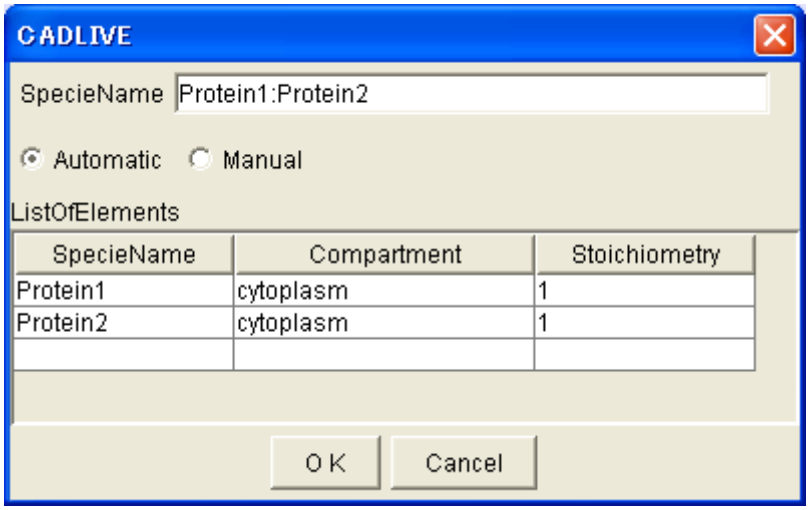
ExchangeComplexReaction denotes exchange reaction (reversible reaction).



When connecting the arrow of "reversible_conversion_in" from TransitionState to a Species, "Set Complex" is displayed. By selecting "Set Complex", the setting dialog for ListOfElements is displayed.

>> ListOfElements setting dialog

The screen for setting the ListOfElements of ExchangeComplex

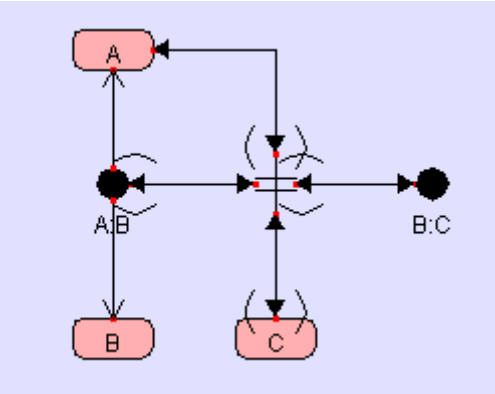


When SpecieName is set as Automatic, ListOfElements that are bound with ":" are displayed.
When SpecieName is set as Manual, SpecieName can be named and edited arbitrarily.

Edit the Combo Box of Spreadsheet, and set the ListOfElements.

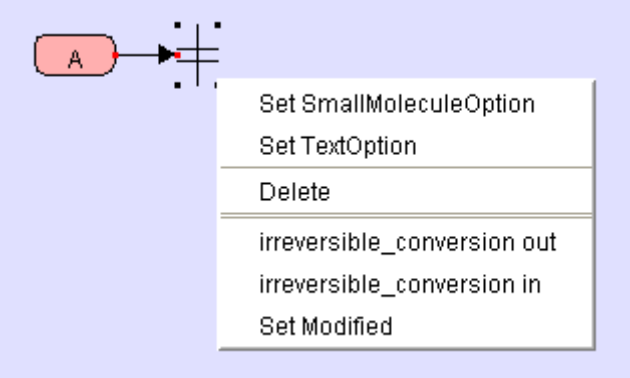
The Species that is a candidate of ListOfElements is Reactants of TransitionState (When Reactants is a Complex/Modified, it contains the ListOfElements of the component.).

By clicking the OK Button, the ExchangeComplexReaction symbol is displayed on NetworkConstructor.



5-2-12 Positioning ExchangeModifiedReaction

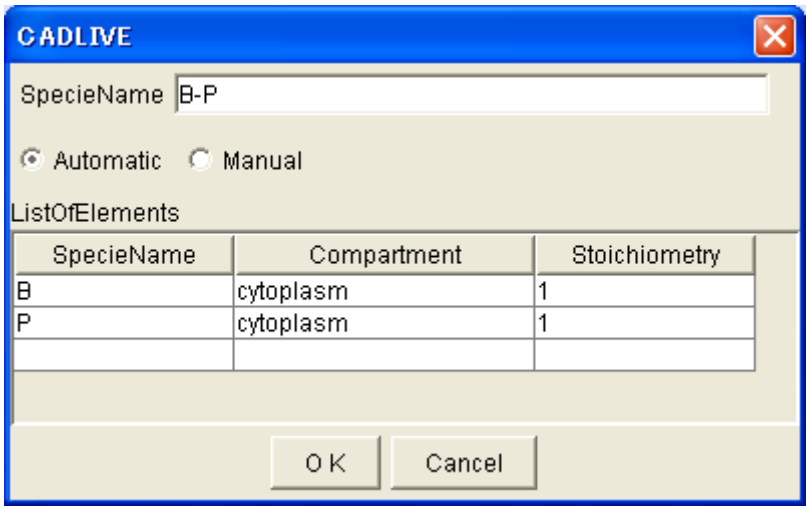
ExchangeModifiedReaction denotes an exchange reaction (irreversible reaction).



When connecting the arrow of "irreversible_conversion_in" from TransitionState to the Species, "Set Modified" will be displayed on the right-click menu. Selecting "Set Modified" displays the setting dialog of ListOfElements.

>> ListOfElements setting dialog

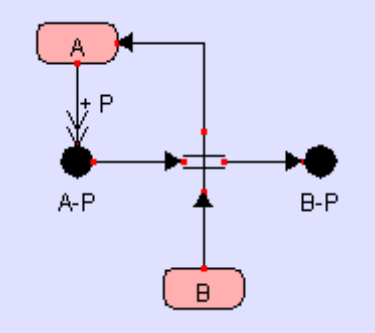
The screen for setting the ListOfElements of ExchangeModifeid.



When SpecieName is set as Automatic, ListOfElements that are connected with “-” are displayed.
When SpecieName is set as Manual, SpecieName can be named and edited arbitrarily.

The Species that is a candidate of ListOfElements becomes Reactants of TransitionState. (When Reactants is a Complex/Modified, it contains the ListOfElements of the component.)

When clicking the OK Button, the ExchangeComplexReaction symbol is displayed on NetworkConstructor.



5-3 Moving Symbol

5-3-1 Moving Species

By dragging a species, it can be moved.
However, TextOption and SmallMoleculeOption cannot move individually.
They move according to the movement of Reaction.

5-3-2 Moving Reaction

By dragging a tip of a Reaction arrow, one can rotate, expand, or contract the arrow while the opposite tip is fixed. However, the arrows attached to TransitionState are not moved for themselves, but moved by dragging TransitionState. The Reaction arrow connected to the Species is moved in accordance with the movement of the Species.

5-3-3 Moving Modifier

By dragging a tip of a Modifier, one can rotate, expand, or contract the Modifier arrows while the opposite tip is fixed. However, the Modifier arrows attached to TransitionState are not moved for themselves, but moved by dragging TransitionState. The Modifier arrow connected to the Species is moved in accordance with the movement of the Species.

5-3-4 Moving Gene

By dragging a Gene, it can be moved. By dragging the tip of the Gene, one can rotate, expand, and contract the reaction arrows while the Gene box is fixed. The Reaction arrow of a Gene connected to a Species is moved together with the movement of the Species.

5-3-5 Moving WhiteBox

By dragging the Symbol viewing area of a WhiteBox, it can be moved.
Despite the movement of a WhiteBox, the symbol stored in the box does not move.

5-3-6 Moving BlackBox

By dragging the Symbol viewing area of a BlackBox, it can be moved.

5-3-7 Moving VirtualReaction

By dragging a tip of VirtualReaction, one can rotate, expand, and contract the Reaction arrow while the opposite tip is fixed.
The VirtualReaction connected to a Species, a Node, or a Domain is moved together with the movement of them.

5-3-8 Moving Domain

By dragging the Domain viewing area of a Domain, it can be moved.
An EquivalenceLine and a Domain partition line are moved together with the Domain.
However, these lines are not allowed to bend.

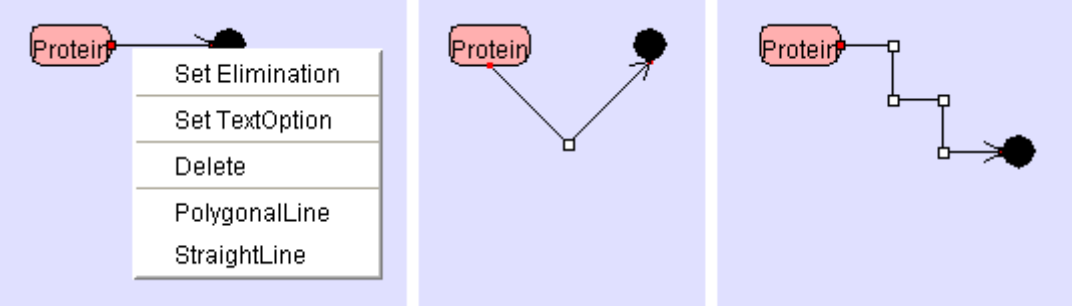
5-3-9 Moving InnnerLink

By dragging a tip of an InnerLink, one can rotate, expand, and contract the arrows while the opposite tip is fixed.
The InnerLink connected to a Species or a Node is moved together with the movement of them.

5-3-10 Moving ExchangeComplexReaction/ExchangeModifiedReaction

By dragging the Symbol viewing area of the Species of ExchangeComplexReaction/ExchangeModifiedReaction, the reaction arrows can be moved.

5-3-11 Bending Symbol

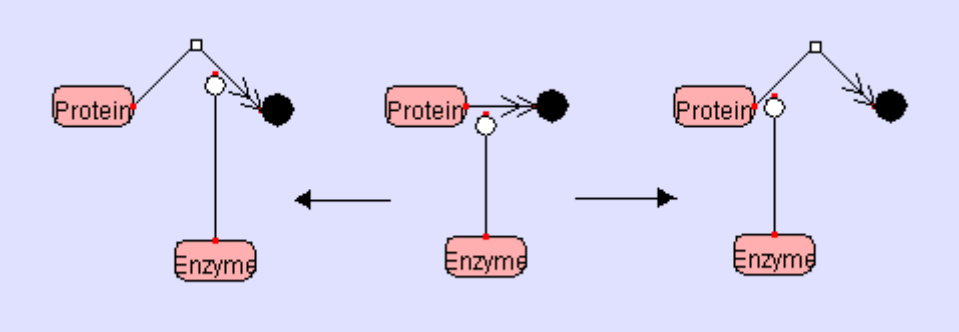


To draw a polygonal line, right-click the line segment that you want to change, and select "PolygonalLine" from the Popup menu.

A handle (□) will appear in the center of the designated line. By dragging the handle, a polygonal line is drawn. A polygonal line can be bent up to 4 times.

To make a polygonal line back to a straight line, right-click the line segment and select "StraightLine" from the Popup menu.

If there is a Modifier attached to the line segment, right-click to draw a polygonal line on the Reactant side. The Modifier will move towards the Product side. Likewise, if one draws a polygonal line by right-clicking on the Product side, the Modifier will move towards the Reactant side.



Right-clicking on the Reactant side Right-clicking on the Product side

5-3-12 Moving multiple symbols simultaneously

By clicking multiple SpeciesSymbols while pushing the Ctrl key and by dragging the selected symbols, one can move SpeciesSymbols simultaneously.

* One neither can select multiple ReactionSymbols nor move them simultaneously.

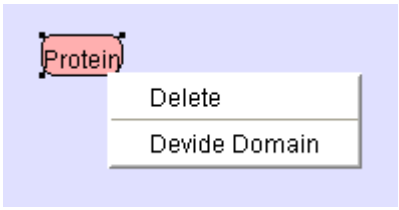
5-3-13 Moving Symbols by using a direction key
One can move Species or Reactions by using the direction key on the keyboard: "$\rightarrow, \leftarrow, \uparrow, \downarrow$". In addition, one can do fine movement by using the direction keys while pushing the Shift key.

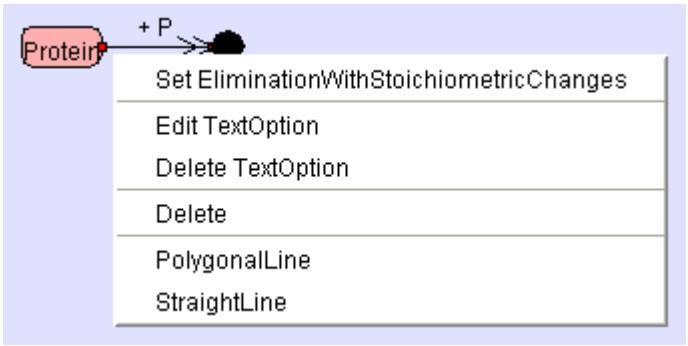
One can move multiple Symbols simultaneously by pushing a direction key while they are selected.

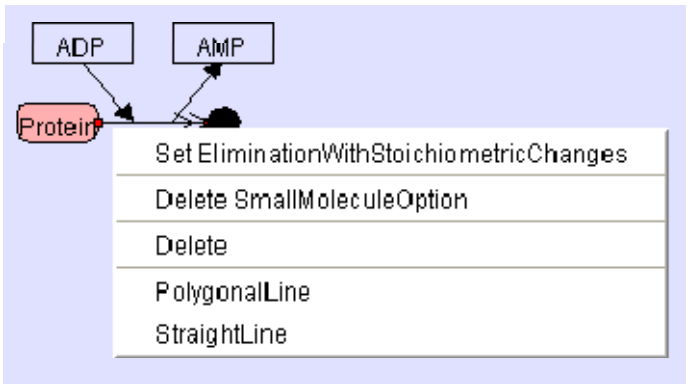
* One cannot move any Reaction connected to a Species.
* One cannot connect a Reaction by using direction keys.

5-4 Deleting Symbol

5-4-1 Deleting Species

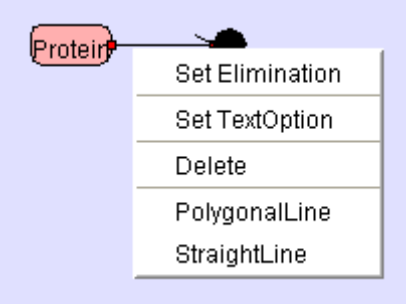






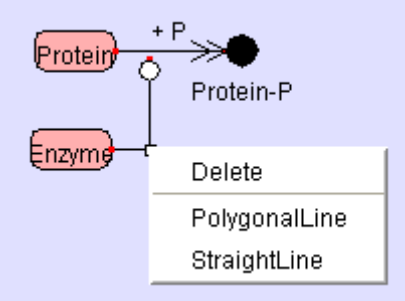
By right-clicking on the Symbol viewing area of the Species and selecting "Delete," the Species is deleted. To delete TextOption or SmallMoleculeOption, right-click the Reaction viewing area where Option has been added, and select "DeleteTextOption" or "DeleteSmallMoleculeOption." When one deletes the Reaction where Option has been added, Option will be deleted simultaneously.

5-4-2 Deleting Reaction



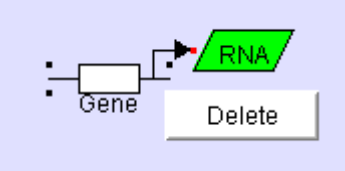
By right-clicking on the Reaction and selecting "Delete," the Reaction is deleted. When both ends of the nodes are connected, Reaction can be deleted by right-clicking the arrow and selecting "Delete."

5-4-3 Deleting Modifier



By right-clicking on a Modifier and selecting "Delete," the Reaction can be deleted. When both ends of the nodes are connected, the Modifier can be deleted by right-clicking the arrow and selecting "Delete."

5-4-4 Deleting Gene



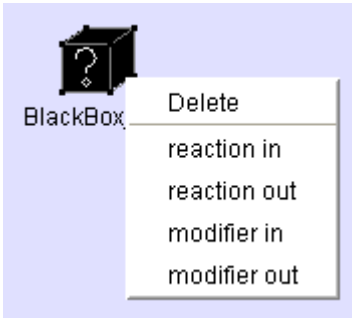
By right-clicking the Species viewing area of a Gene and selecting "Delete," the Gene is deleted. However, one cannot delete it by right-clicking the Reaction area.

5-4-5 Deleting WhiteBox

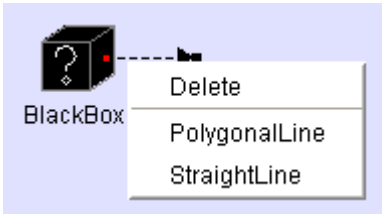
A WhiteBox should be deleted on the WhiteBoxTreeWindow.

5-4-6 Deleting BlackBox

By right-clicking on the viewing area of a BlackBox and selecting "Delete," the BlackBox is deleted. When deleting a BlackBox, all the unknownReaction/unknownModifiers that are connected to the BlackBox are deleted together.

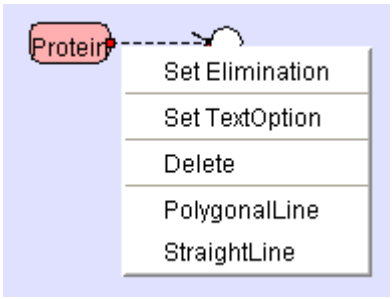


>> Deleting the unknownReaction/unknownModifier



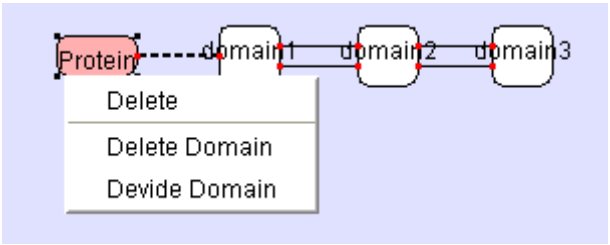
By right-clicking a unknownReaction/unknownModifier and selecting "Delete," the unknownReaction/unknownModifier is deleted.

5-4-7 Deleting VirtualReaction



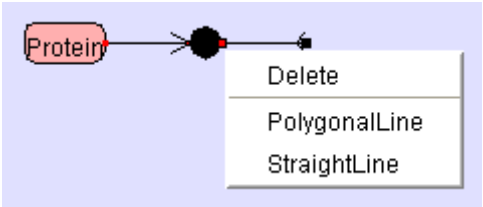
By right-clicking a VertualReaction and selecting "Delete," the VertualReaction is deleted.

5-4-8 Deleting Domain



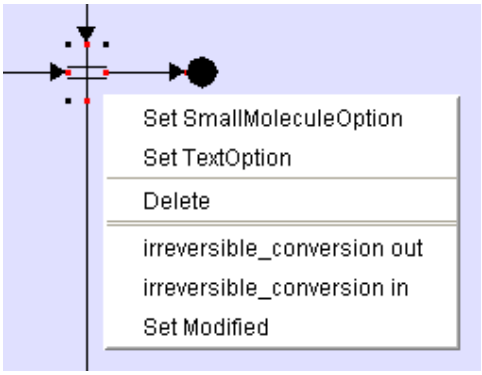
When deleting the entire Domain, select "Delete Domain" from the right-click menu of the Species of an origin of link. When deleting a specific Domain, select "Divide Domain" to edit in DomainDialog.

5-4-9 Deleting InnerLink



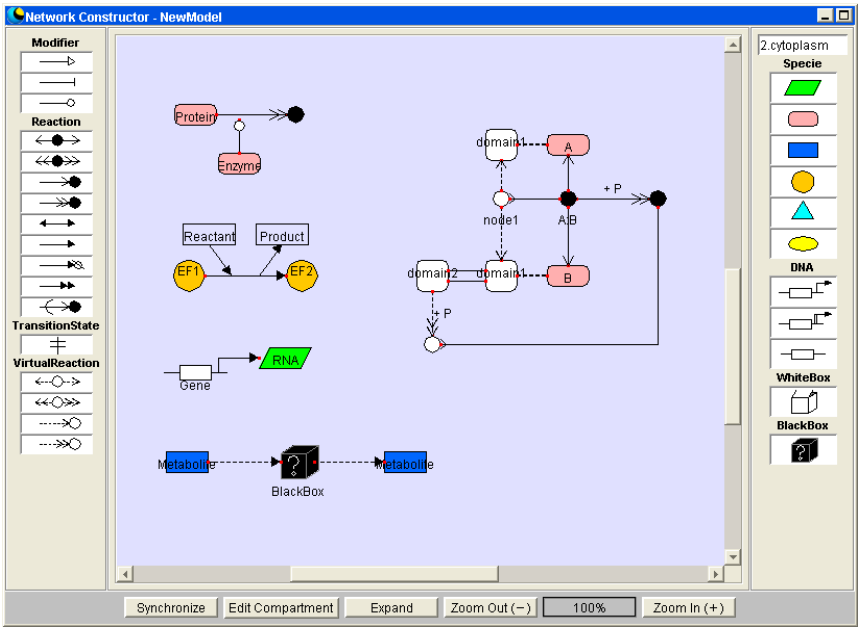
By right-clicking an InnerLink and selecting "Delete," the InnerLink is deleted.
When deleting the Species of an origin of link, the InnerLink is deleted simultaneously.

5-4-10 Deleting ExchangeComplexReaction/ExchangeModifiedReaction



By right-clicking an ExchangeComplexReaction/ExchangeModifiedReaction and selecting "Delete," the Reaction is deleted. When deleting the TransitionState of an origin of links, the ExchangeComplexReaction/ExchangeModifiedReaction is deleted simultaneously.

5-5 Connecting Symbol



5-5-1 Connecting Reaction, Modifier, VirtualReaction and Species

By dragging a tip of a Reaction or Modifier onto the Symbol of a Species, the Reaction or Modifier is connected with the Species.

Both ends of the arrows turn red in color when the Species is successfully connected to the Reaction or Modifier.

*The BlackBox symbol is treated in the same manner as the other Species symbols.

5-5-2 Connecting Gene and Species

By dragging the tip of Transcription and Protein_synthesis onto the Symbol of a Species, DNA (Transcription, Protein_synthsis) and the Species are connected.

5-5-3 Connecting Modifier and Reaction

By dragging a tip of a Modifier onto a Reaction or another Modifier 's arrow, they are connected.

* One cannot connect a tip of a Modifier to a reversible reaction. Instead of the reversible reaction, two irreversible reactions should be used.

5-5-4 Connecting VirtualReaction, VirtualNode and Domain

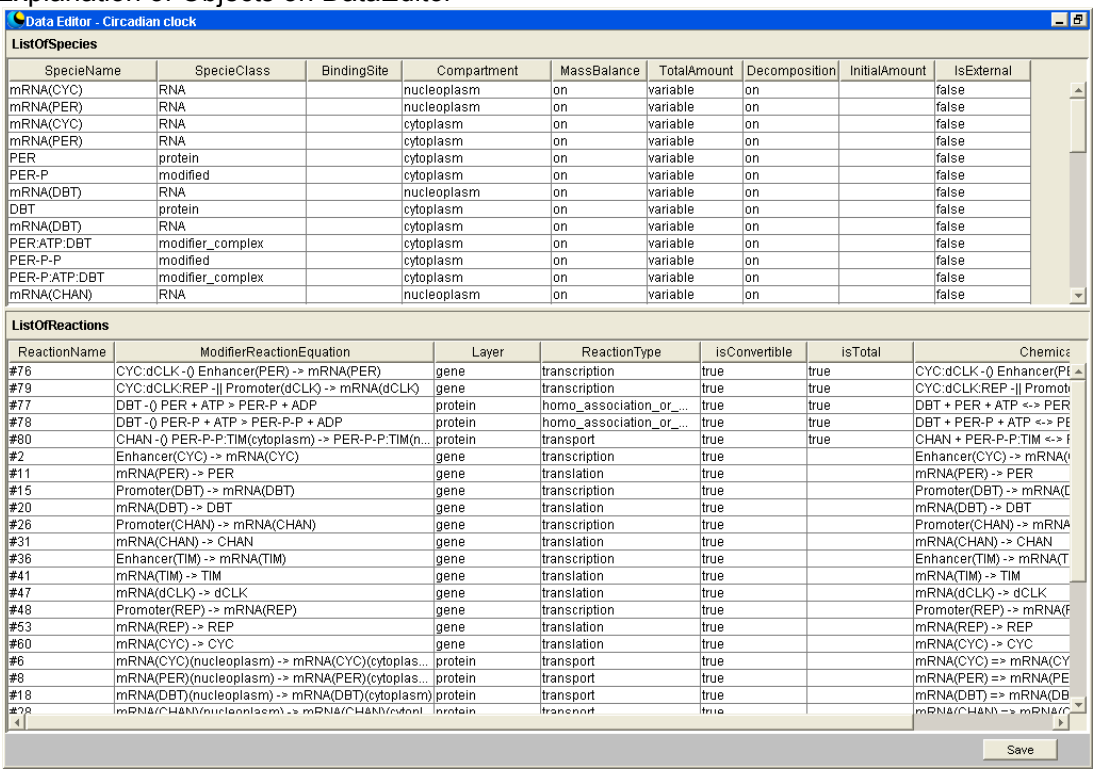
By dragging a tip of VirtualReaction onto a Species, a VirtualNode, or a Domain, they are connected.

5-5-5 Connecting InnerLink, Species and VirtualNode

By dragging a tip of InnerLink onto a Species or VirtualNode, they are connected.

6. Data Editor

6-1 Explanation of Objects on DataEditor



6-1-1 Species Spreadsheet

This is the spreadsheet used to display, input, and edit the attribute data of Species and BlackBox positioned by NetworkConstructor. Before inputting texts, make sure that the input cell is "selected." After inputting text, press the return key to define it.

6-1-2 Reaction Spredsheet

This is the spreadsheet to display, input, and edit the attribute data of Reaction positioned by NetworkConstructor. Before inputting text, make sure that the cell to input data is "selected." After inputting text, press the return key to define it.

6-1-3 Save Button

The XML file created by NetworkConstructor or DateEditor will be saved in the model folder (C: ¥CADLIVE¥data¥model). It is the same function as "Save" in the File menu.

6-2 Explanation of Specie Items

>> SpecieName

The Species positioned will be given as a temporary name in the system, which can be edited by DataEditor.

The name connecting the SpecieName with colons like "A:B:" is given as a Complex; the name connecting SpecieName with hyphens like "A-B-" is given as a Modified. Such rules cannot be changed.

>> SpecieClass

"SpecieClass" denotes the material attributes of Species generated by NetworkConstructor.

DNA
RNA
protein
metabolite
environmental_factor
ion_signal
complex
modifier_complex (Enzyme-substrate complex: This name is automatically created by the system, cannot be edited by users)
modified (Modified Substance)
text_option (Specie Generated by a text_option)
small_molecule_option (Specie Generated by a small_molecule_option)
others
black_box

>> BindingSite
"BindingSite" denotes the classification of the DNAs that neither encode any protein nor RNAs as a material attribute.
enhancer : activating factor binding site of DNAs.
promoter : inhibiting factor binding site of DNAs.
other : non-specific binding sites of DNAs
The default is other. Depending on the selection box, the displayed content can be changed.

>> Compartment
"Component" denotes the location attributes of Species generated by NetworkConstructor.
environment
cytoplasm
nucleoplasm
ER
mitochondria
golgi
chloroplast
membrane
other

* Despite the position of WhiteBox, the Compartment of Species and BlackBox stored in WhiteBox is set as the same Compartment as defined initially.

>> MassBalance
Select a MassBalacne attribute in the ListOfSpecies.
off : It does not require any mass balance equation.
on : It requires a mass balance equation.
When the SpecieClass is DNA_promoter, DNA_enhancer, DNA_other, Protein, Modified, the default is "on," if not, the default is "off."
The viewing content can be changed using the selection box.
Regarding BlackBox, a blank is displayed, and it cannot be edited.

>> TotalAmount
Select a TotalAmount attribute in the ListOfSpecies.
constant : constant in mathematical equations
variable : variable in mathematical equations
If the SpecieClass is DNA, metabolite, environmentl_factor, ion_sygnal, small_molecule and other, the default is “constant”. If not, the default is "variable".

Depending on the selection box, the displayed content can be changed.
Regarding BlackBox, a blank is displayed, and it cannot be edited.

>> Decomposition
Select a Decomposition attribute in the ListOfSpecies.
on : generates the decomposition term in a mathematical model
off : does not generate the decomposition term in a mathematical model
When the SpecieClass is RNA, Protein, Metabolite, Complex or Modified, the default is "on," if not, the default is "off." The viewing content can be changed using the selection box.
Regarding BlackBox, a blank is displayed, and it cannot be edited.

>> InitialAmount
Input the initial value of a species.
Note that users are not allowed to edit BlackBox. A blank is displayed.

>> IsExternal
Select an IsExternal attribute of a Species.
If the isExternal of Specie is "True", the Specie is not affected by gene knockout.
Users are not allowed to edit "IsExternal" of Complex, Modified, and ModifierComplex.

6-3 Explanation of Reaction Items

>> ReactionName
The Reaction name is displayed that is attached by the symbol “#” preceding Reaction ID.

>> ModifierReactionEquation
The regulator reaction equations corresponding to the map are displayed. (They appear in the order of Modifier Species, ModifierType, ReactantReaction Species, Reaction, and ProductReaction Species.)

>> Layer
Select the reaction layer.
metabolic : reaction at the metabolic layer
protein : reaction at the protein interaction layer
gene : reaction at the gene expression layer
The default is given according to ReactionType.
The viewing content can be modified using the selection box.

>> ReactionType
Reaction attributes generated by NetworkConstructor are displayed.
binding
binding_with_stoichiometric_changes
homo_association_or_modification
homo_association_or_modification_with_stoichiometric_changes
elimination
elimination_with_stoichiometric_changes
reversible_conversion
irreversible_conversion
reversible_conversion_regarding_multicompornent
irreversible_conversion_regarding_multicompornent
transport
option_transport
transcription

translation
degradation
activation_of_specie
inhibition_of_specie
activation_of_modifier
inhibition_of_ modifier
unknown_reaction
unknown_modification_of_modifier
unknown_modifier_of_specie

>> isConvertible
"isConvertible" determines if the CADLIVE simulator converts the reaction into mathematical equations or not.
true : It is convertible.
false : It is not convertible.
The default is true.
Depending on the selection box, the displayed content can be changed.
Note that the reaction that is not able to be converted into any regulator reaction equation is “false”, and it cannot be changed by users.

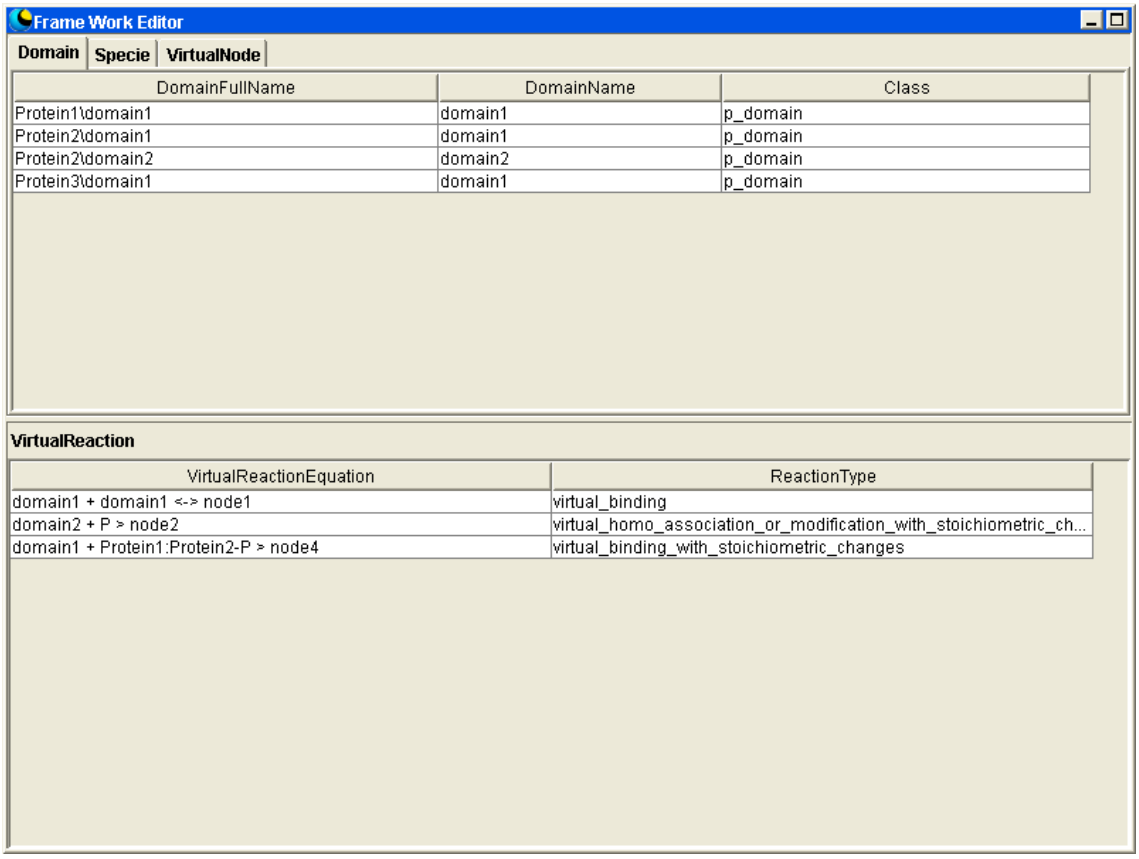
>> isTotal
Select how to calculate the amount of modifiers by the CADLIVE simulator.
true : the modifier concentration is the Total amount
false : the modifier concentration is the free modifier amount.
The default is true.
Depending on the selection box, the displayed content can be changed.

>> ChemicalReactionEquation
Displays chemical reaction equations of the Reaction.
The reaction whose attribue of "isConvertible" is “false” does not create any ChemicalReactionEquation.

7. Framework Editor

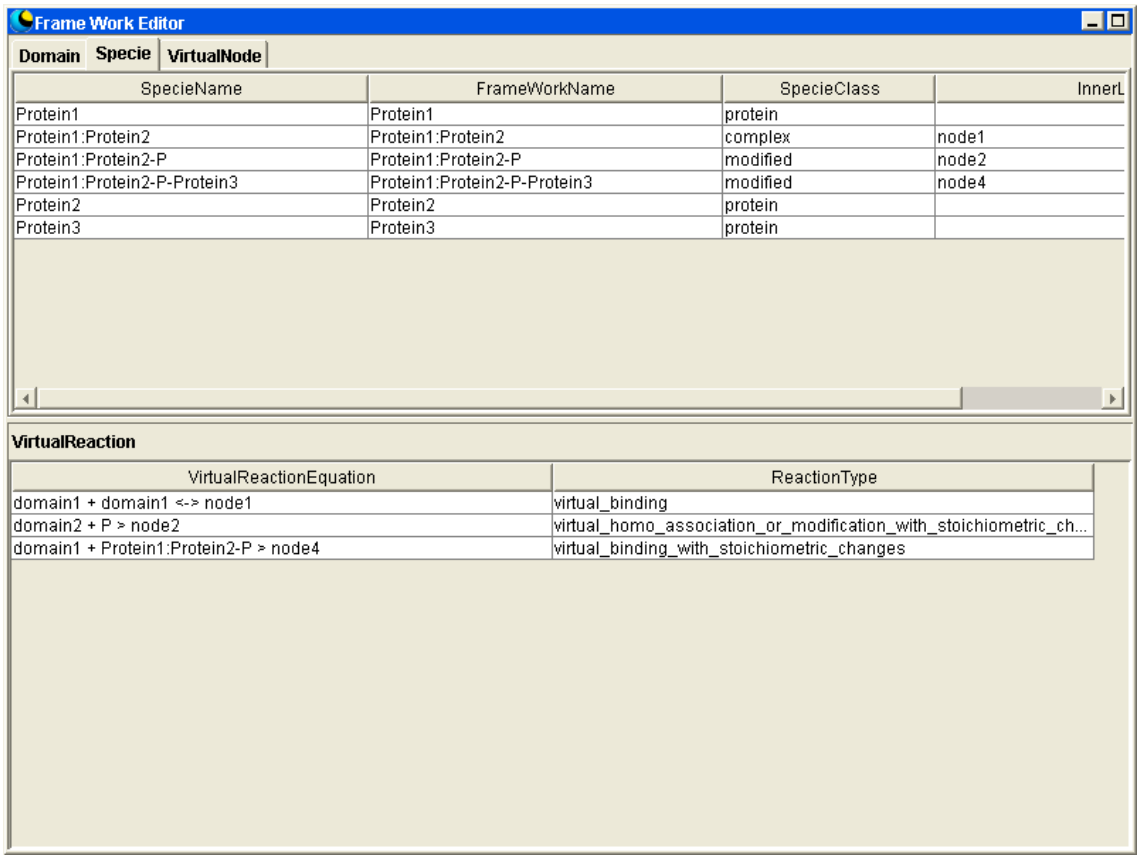
7-1 Explanation of Objects on Framework Editor

7-1-1 Domain Spreadsheet



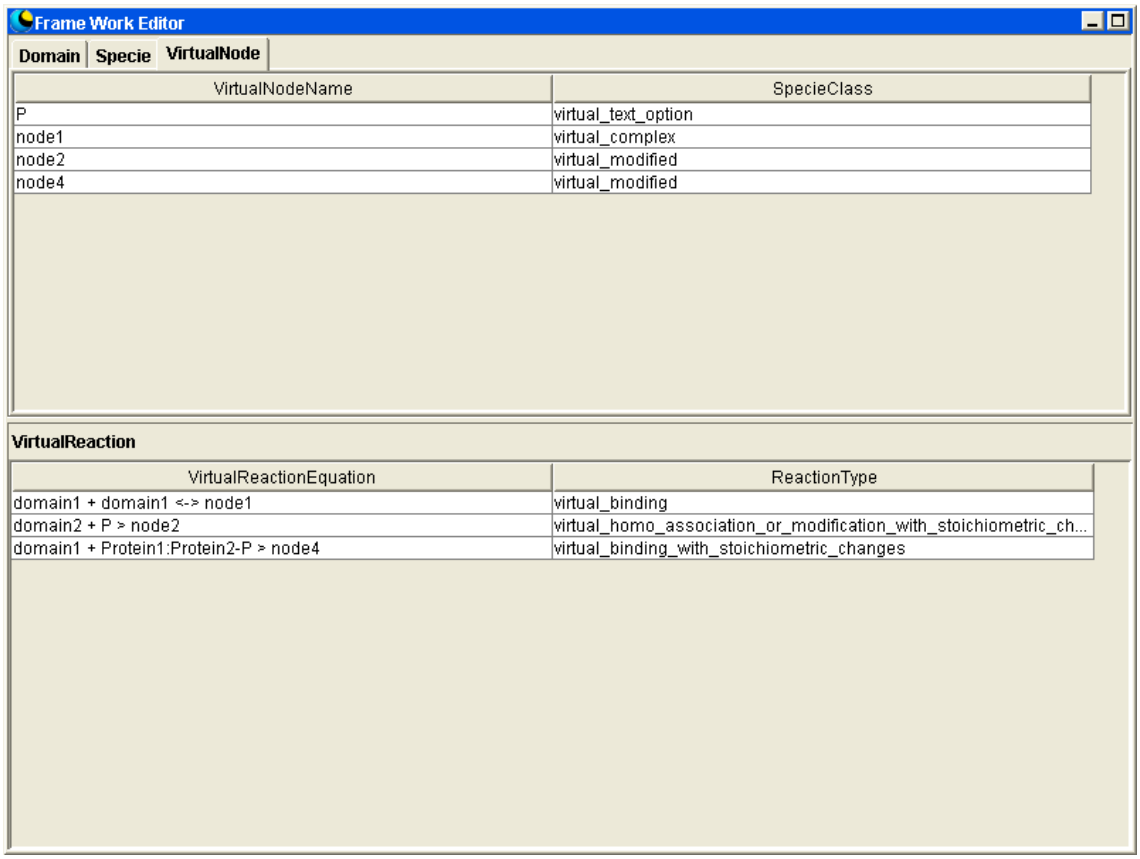
This is the spreadsheet used to display, input, and edit the attribute data of the Domain positioned by NetworkConstructor. Before inputting texts, make sure that the input cell is "selected." After inputting text, press the return key to define it.

7-1-2 Species Spreadsheet



This is the spreadsheet used to display, input, and edit the attribute data of the Species that involves BuildingFramework out of the Species placed by NetworkConstructor. Before inputting texts, make sure that the input cell is "selected." After inputting text, press the return key to define it.

7-1-3 VirtualNode Spreadsheet



This is the spreadsheet used to display, input, and edit, the attribute data of the VirtualNode positioned by NetworkConstructor. Before inputting texts, make sure that the input cell is "selected." After inputting text, press the return key to define it.

7-1-4 VirtualReaction Spreadsheet

This is the spreadsheet used to display, input, and edit the attribute data of the VirtualReaction positioned by NetworkConstructor. Before inputting texts, make sure that the input cell is "selected." After inputting text, press the return key to define it.

7-2 Explanation of Domain Items

>> DomainFullName
DomainFullName denotes the name of Domain with the name of the Species of the origin of division.

>> DomainName
Domain denotes the names of the Domain, which is allowed to be edited.

>> Class
Class denotes the material attribute of Domain.
r_domain
p_domain

7-3 Explanation of Species Items

>> SpecieName
SpecieName denotes the name of a Species.

>> FrameworkName
FrameworkName gives the name peculiar to BuildingFramework to Species. Users are allowed to edit it.

>> SpecieClass
SpecieClass denotes the material attributes of a Species.
RNA
protein
complex
modified

>> InnerLink
InnerLink denotes the Species and Nodes that are connected by InnerLink.
When there are multiple targets bound by InnerLinks, divide them with "//" and display it.

7-4 Explanation of VirtualNode Items

>> VirtualNodeName
VirtualNodeName denotes the name of VirtualNode. Users are allowed to edit it.
Unlike the case of Species, "virtual_complex" and "virtual_modified" are not named automatically.

>> SpecieClass
SpecieClass denotes the material attributes of VirtualNode.
virtual_complex
virtual_modified
virtual_text_option (Node Species generated by a text_option)
virtual_small_molecule (Node Species generated by a text_option)

7-5 Explanation of VirtualReaction Items

>> VirtualReactionEquation
VirtualReactionEquation denotes the regulaor-reaction equation of the VirtualReaction created by NetworkConstructor.

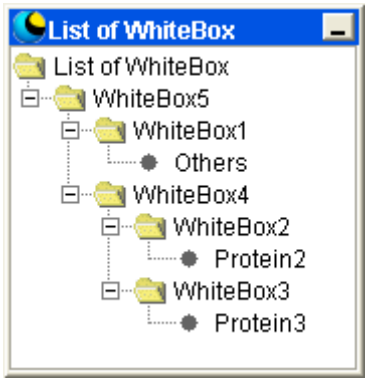
>> ReactionType
ReactionType denotes the reaction attributes of the VirtualReaction created by NetworkConstructor.

virtual_binding
virtual_binding_with_stoichiometric_changes
virtual_homo_association_or_modification
virtual_homo_association_or_modification_with_stoichiometric_changes
virtual_elimination
virtual_elimination_with_stoichiometric_changes

8. WhiteBoxTreeWindow

8-1 WhiteBoxTreeWindow screen

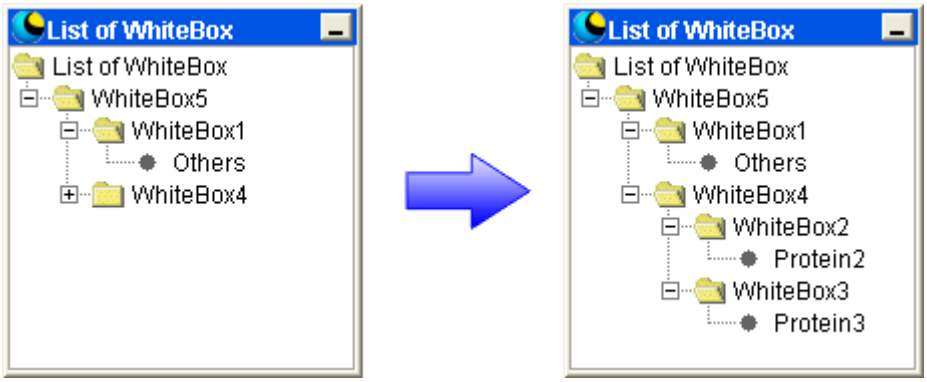
Display of the content of WhiteBox in a tree structure.



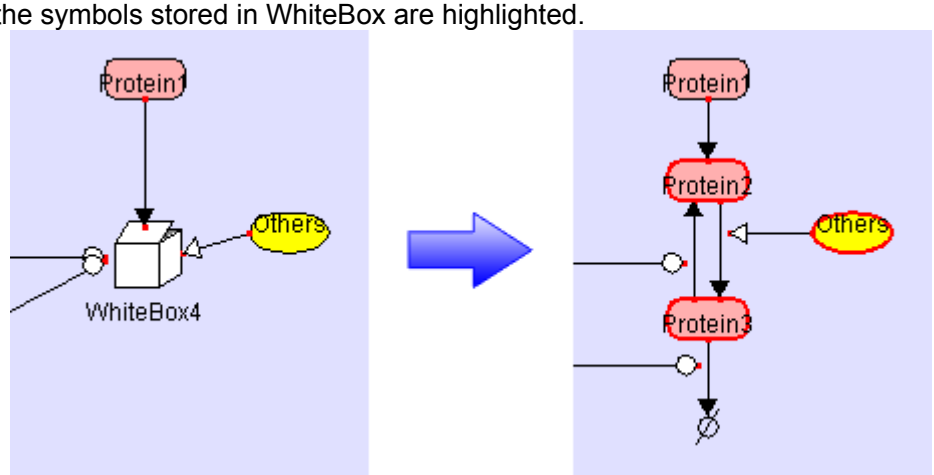
8-2 Operation of WhiteBoxTreeWindow

8-2-1 Expanding WhiteBox

By clicking "+" in the left of WhiteBox, WhiteBox is expanded.
At the same time, the WhiteBox on a panel is expanded and is displayed.

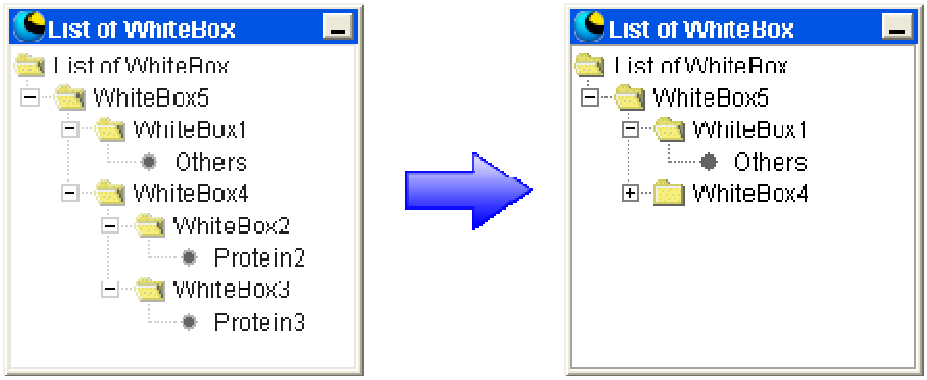


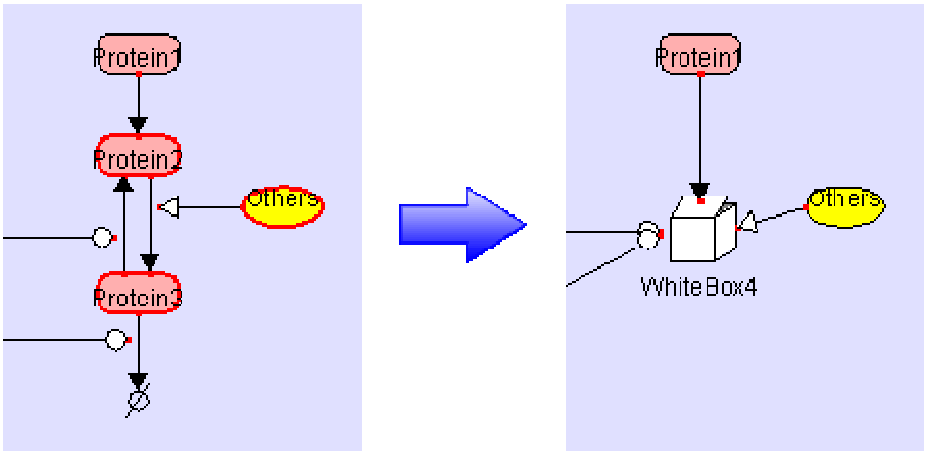
>> highlight the symbol
All the symbols stored in WhiteBox are highlighted.



8-2-2 Storing WhiteBox

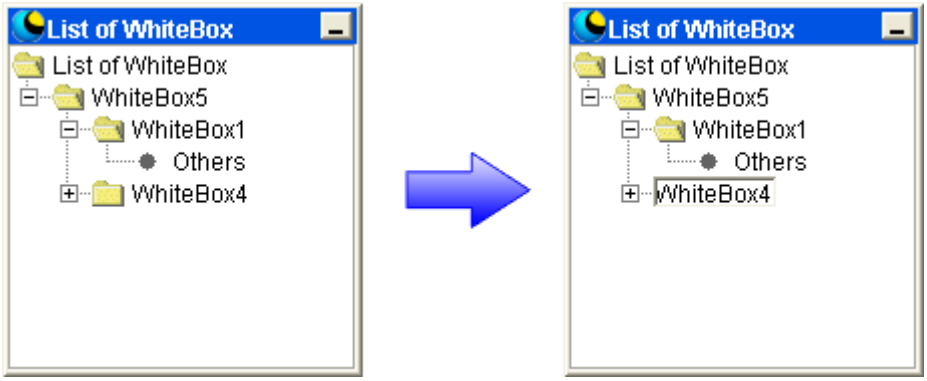
By clicking "-" in the left of WhiteBox, the Species are stored in the WhiteBox.
At the same time, the WhiteBox on a panel stores the Species.





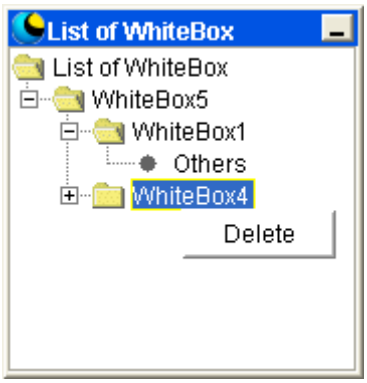
8-2-3 Editing the name of WhiteBox

Double-click the folder-type icon or the name of WhiteBox to edit.
Before inputting text, make sure that the cell to input data is "selected." After inputting text, press the return key to define it.
Users are not allowed to rename Species or VirtualNode from WhiteBoxTreeWindow.
The names of Species and VirtualNode should be renamed on DataEditor and on FrameworkEditor, respectively.



8-2-4 Deleting the WhiteBox

By right-clicking on the WhiteBox to delete and selecting "Delete," the WhiteBox is deleted.
The symbols stored in the deleted WhiteBox moves to a one-layer upper level.
Users are not allowed to delete the Species or VirtualNode from WhiteBoxTreeWindow.
Delete the Species and VirtualNode on a panel.

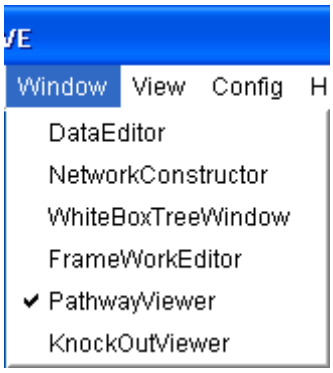


9. PathwayViewer

Depending on the machine spec. to be used, trouble may occur in operation of PathwayViewer.

9-1 Start-Up of PathwayViewer

9-1-1 Start-up on CADLIVE

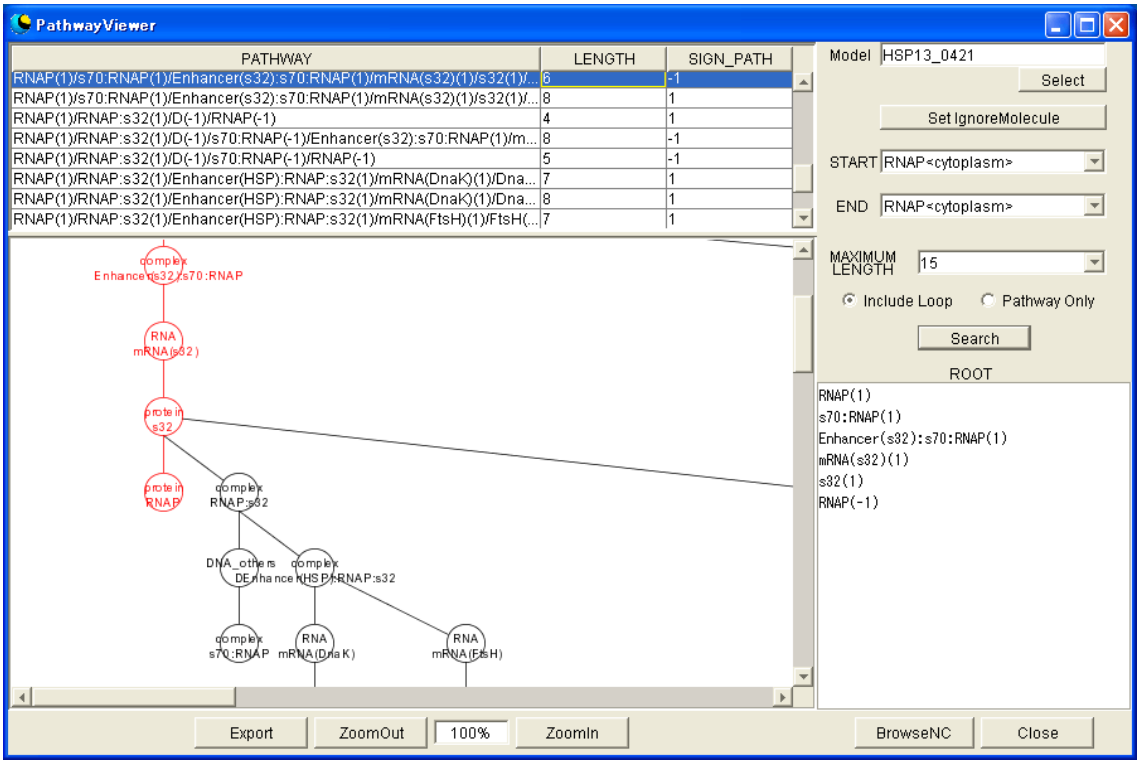


In order to start PathwayViewer from CADLIVE, select PathwayViewer of the Window menu while opening the model on the screen. During this process, the model network is automatically saved in the system.
When start-up on CADLIVE, users are able to search the pathways and highlight the resultant pathways on NetworkConstructor.

9-1-2 Start-up in a single PathwayViewer

Make sure that Java™ 2 Runtime Environment (**1.3**) has been installed.
Select PATHWAY from the Program menu or double-click the "PATHWAY.exe" on the directory (C:¥CADLIVE) where CADLIVE is installed.
When start-up in the single PathwayViewer, users are not able to work together with CADLIVE (highlighting the pathway on NetworkConstructor).

9-2 Explanation of Objects on PathwayViewer



9-2-1 Model

Display the current Model name.

9-2-2 Set IgnoreMolecule Button

Set the molecules to ignore in a pathway search.

9-2-3 Select Button

Read new Model (an XML file that describes regulator-reaction equations in the sanac format).
*When reading a new model, the highlight display with the BrowseNC button is disabled.

9-2-4 Start Combo Box

This is the combo box to select the Species that is the starting point of a pathway search.
*In the combo box, the Species list of the current model are displayed.
The Species that are ignored are not displayed in the list.

9-2-5 End Combo Box

This is the combo box to select the Species that is the terminal point of a pathway search.
*In the combo box, the Species list of the current model is displayed.
The Species that are ignored are not displayed in the list.

9-2-6 MaximumLength Combo Box

This is the combo box to select the length of the pathway search. Length can be set to

999 at the maximum.
*When the number increases, the pathway search may fail and will require a long calculation time.

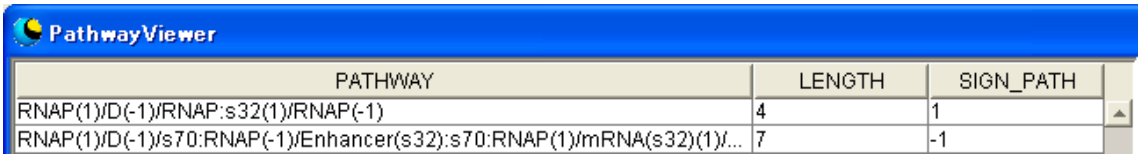
9-2-7 Include Loop Radio Button
When selecting "Include Loop", the pathways including local loops are explored.

9-2-8 Pathway Only Radio Button
When selecting "Pathway Only", the pathways excluding local loops are explored.

9-2-9 Search Button
The pathway search is carried out under the conditions shown in the Start combo box, End combo box, and MaximumLength combo box.
*When lots of search results are produced, operations may stop temporarily.

9-2-10 ROOT Panel
The Species that exist on the pathways selected in the Pathway spreadsheet are displayed in order.

9-2-11 Pathway Spreadsheet
The results of pathway search are displayed in the spreadsheet.



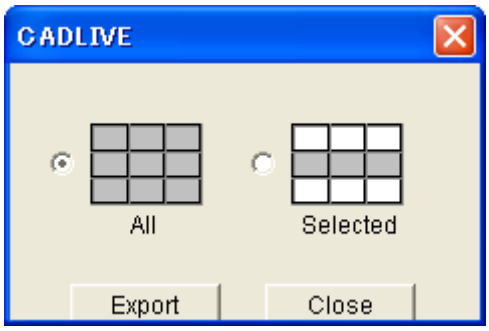
>> PATHWAY
The pathways that are divided by slashes are displayed.

>> LENGTH
The length from the starting point to the terminal point of a pathway is displayed.

>> SIGN_PATH
The "SIGN_PATH" of a pathway displayed with "1" or "-1".

9-2-12 Tree Panel
The result of the search is displayed in a tree structure, where the pathway selected in the pathway spreadsheet is shown as a main stem, and the looped pathways as branches.

9-2-13 Export Button



The results in the pathway spreadsheet are exported in a CSV format.

When selecting "All", the whole data in the pathway spreadsheet is exported.
When selecting "Selected", the data of the selected lines in the pathway spreadsheet is exported.

9-2-14 Zoom Out Button

Clicking this button will reduce the viewing area of the Tree panel (Individual Symbols will be reduced accordingly.)
The area can be zoomed out up to 25%.

9-2-15 Zoom In Button

Clicking this button will expand the viewing area of the Tree panel (Individual Symbols will be enlarged accordingly.)
The area can be zoomed in up to 400%.

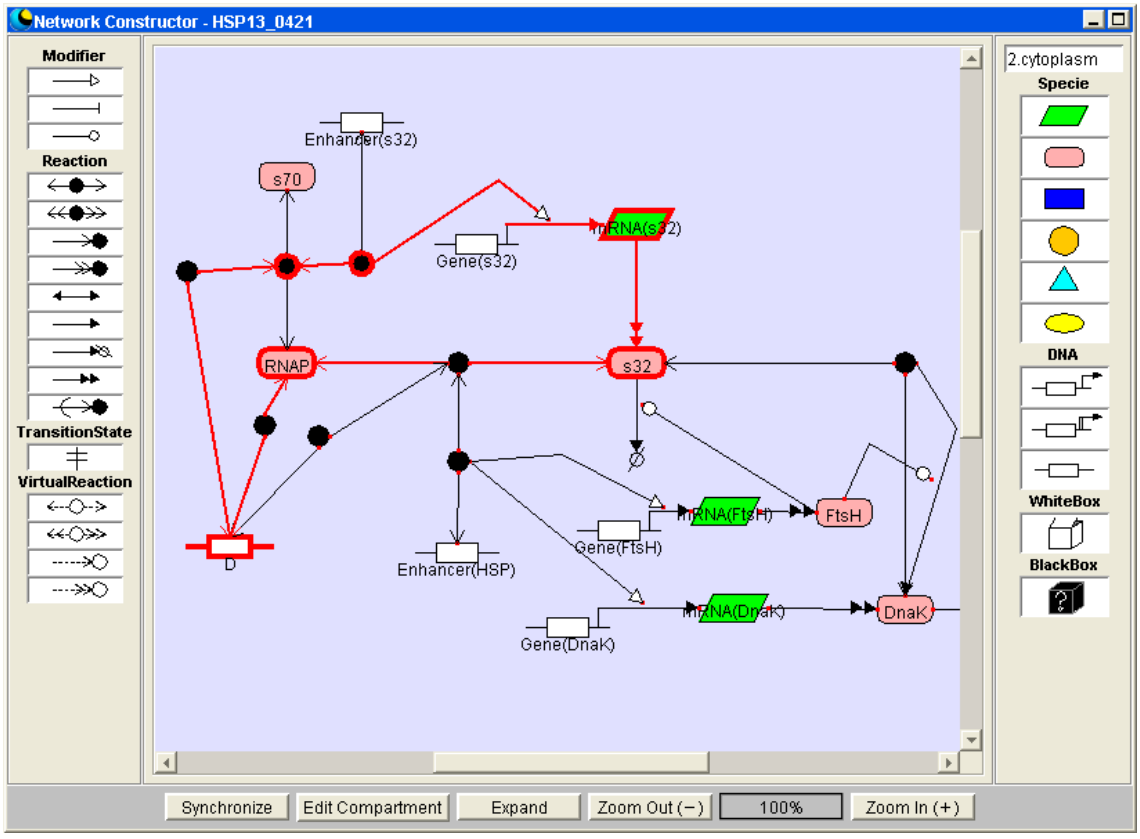
9-2-16 Zoom Magnification Display Box

The box displays the current zoom magnification.

9-2-17 BrowseNC Button

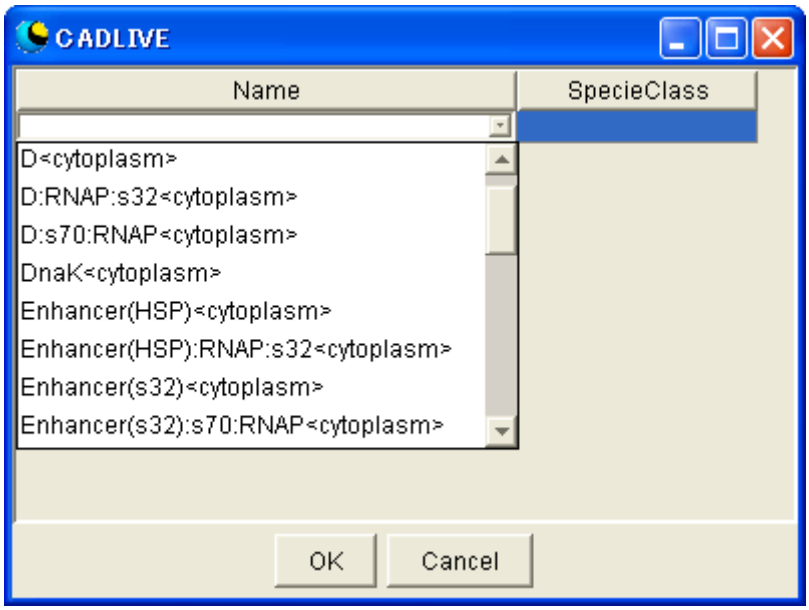
Cliking "BrowseNC" highlights the pathway selected in the pathway spreadsheet on NetworkConstructor.

*It is required to read the same model as displayed on CADLIVE in PathwayViewer in order to highlight a pathway.
When mismatches occur in both models, this function does not work.
If users use a pathway search using NetworkConstructor, finish PathwayViewer, and start-up from CADLIVE.



9-2-18 Close Button
Close PathwayViewer

9-3 Explanation of objects of the screen setting the molecules to ignore



This is the screen for setting the molecules to ignore on a pathway search.

9-3-1 Spreadsheet

This is the screen for setting the molecules to ignore from a pathway search.
Select the Species to ignore from the select box.

*All Species registered in a model are stored in a select box.
*By selecting the blank on a select box, the molecule is deleted.

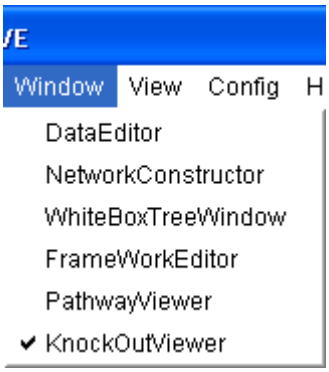
9-3-2 OK Button
Setting the Species that is selected as the molecule to ignore

9-3-3 Cancel Button
Editing is canceled and a screen is closed.

10. KnockOutViewer

10-1 Start-Up of KnockOutViewer

10-1-1 Start-up on CADLIVE

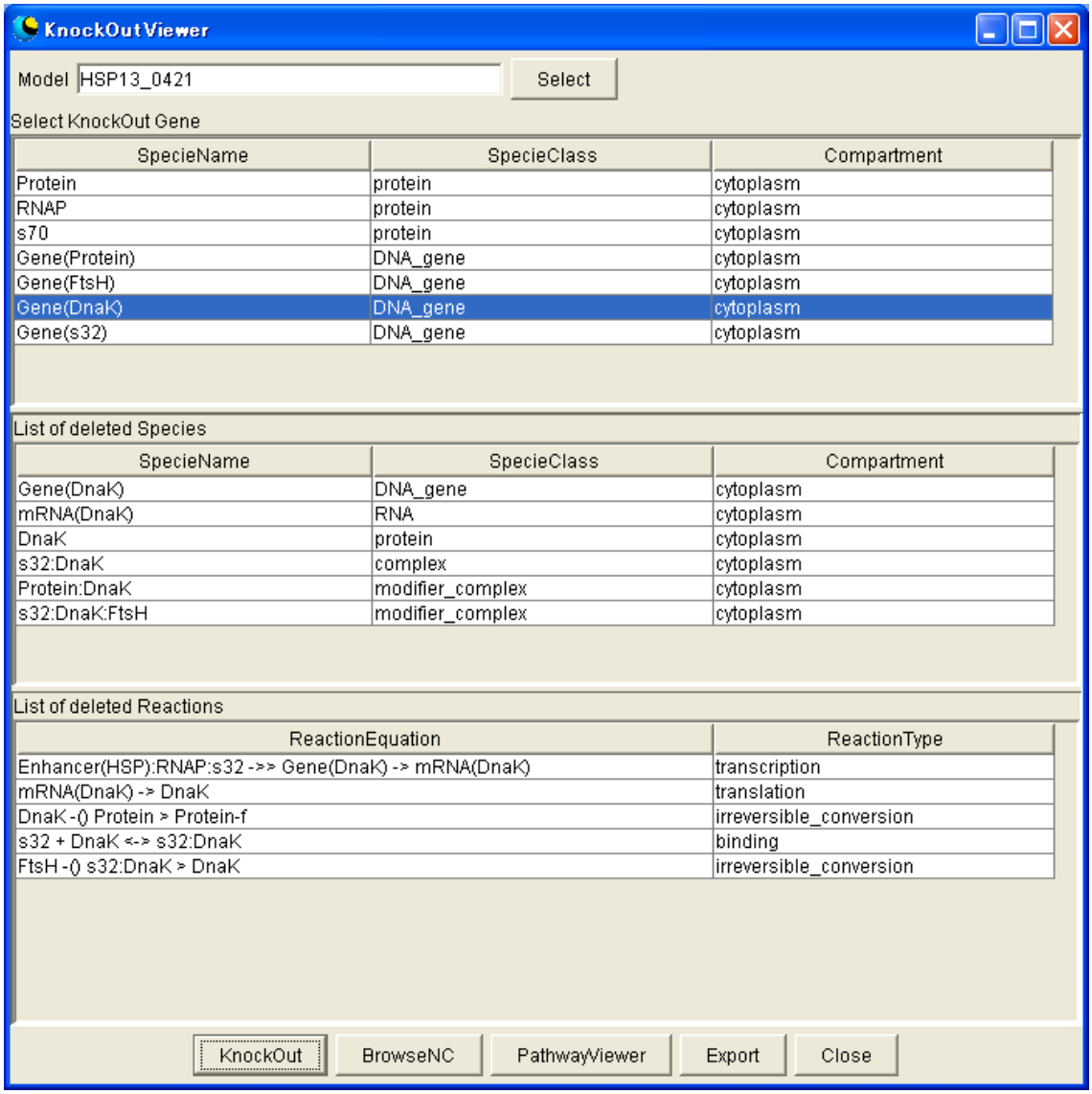


In order to start KnockOutViewer from CADLIVE, select PathwayViewer of the Window menu, while opening the model on the screen. During this process, the model network is automatically saved in the system.
When start-up on CADLIVE, users are able to search the pathways and highlight the results on NetworkConstructor.

10-1-2 Start-up in single KnockOutViewer

Make sure that Java™2 Runtime Environment (1.3) has been installed.
Select KNOCKOUT from the Program menu or double-click the "KNOCKOUT.exe" on the directory (C:¥CADLIVE) where CADLIVE is installed.
When start-up the single KnockOutViewer, users are not able to work together with CADLIVE (highlighting the pathway on NetworkConstructor).

10-2 Explanation of Objects on KnockOutViewer



10-2-1 Model

Display a current Model name.

10-2-2 Select Button

Read a new model (an XML file that describes regulator-reaction equations in the sanac format).
*When reading a new model, the highlight display by the BrowseNC button is disabled.

10-2-3 Select KnockOut Gene Spreadsheet

This is the spreadsheet to select the Gene to knockout.
When selecting the multiple species, click the rows pushing the Ctrl key.
By selecting multiple raws, selected Genes are eliminated simultaneously.

*On the Gene of the object of KnockOut, the Species whose SpecieClass is Gene_DNA and the Species whose SpecieClass is RNA/Protein and IsExternal is true are displayed.

10-2-4 ListOfDeletedSpecies Spreadsheet

This is the spreadsheet that displays the list of the deleted Species after pressing the KnockOut button.

10-2-5 ListOfDeletedReactions Spreadsheet

This is the spreadsheet that displays the list of the deleted Reactions after pressing the KnockOut button.

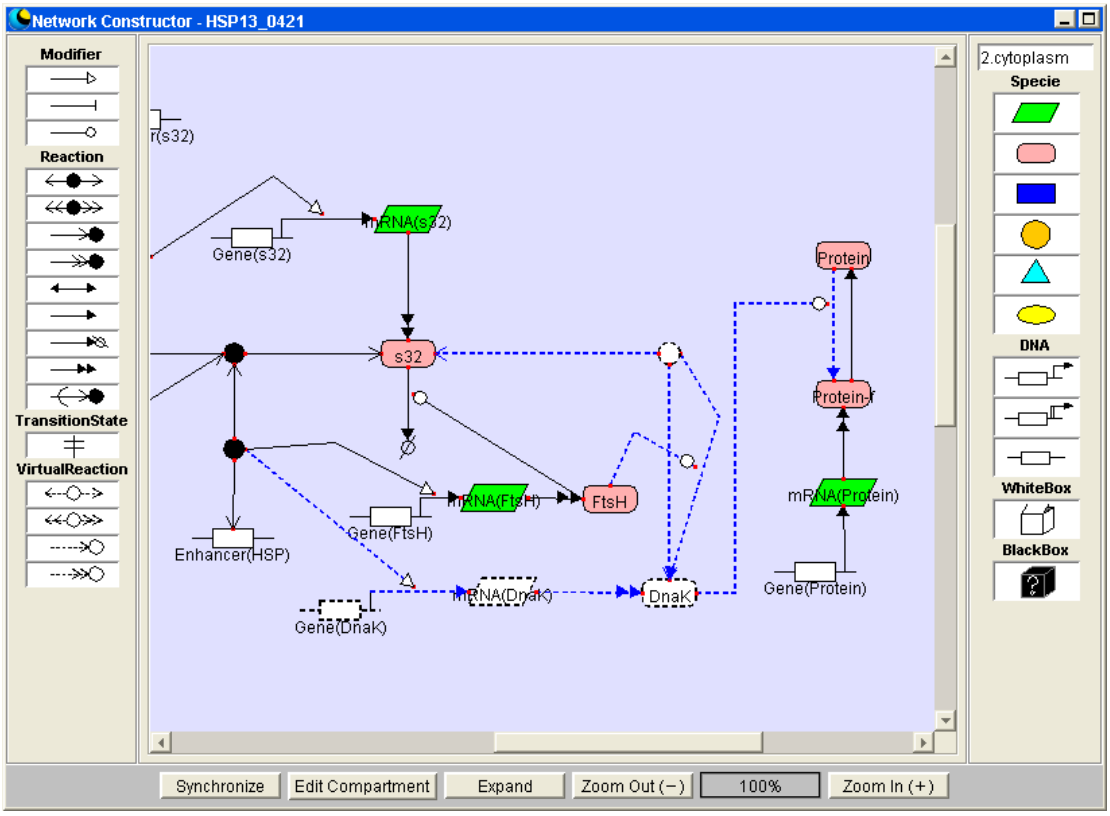
10-2-6 KnockOut Button

Users carry out KnockOut of Gene selected on a SelectKnockOutGene spreadsheet. KnockOut results are displayed on ListOfDeletedSpecies spreadsheet and ListOfDeletedReactions spreadsheet.

10-2-7 BrowseNC Button

It highlights (dashed line) the deleted Species and Reactions on NetworkConstructor.

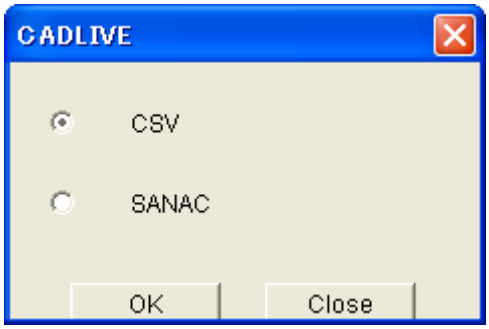
*It is required to read the same model as displayed on CADLIVE in KnockOutViewer in order to highlight a pathway.
When reading a new Model, this function does not work.
If users like to see knockout results on NetworkConstuctor, start-up from CADLIVE



10-2-8 PathwayViewer Button

Start-up the PathwayViewer. By pressing the PathwayViewer button after running the Knockout, users can carry out a pathway search for the knockout network.

10-2-9 Export Button



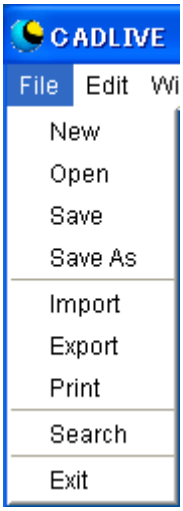
Results of knockout will be exported as CSV format and SANAC(XML) format.
When selecting the CSV format, KnockOut results will be exported as the CSV format.

10-2-10 Close Button

Close KnockOutViewer.

11. Explanation of Menu Items

11-1 File Menu



11-1-1 New

Start the NewDialog box.
Positioning the Compartment in the dialog box. (4-2)

11-1-2 Open

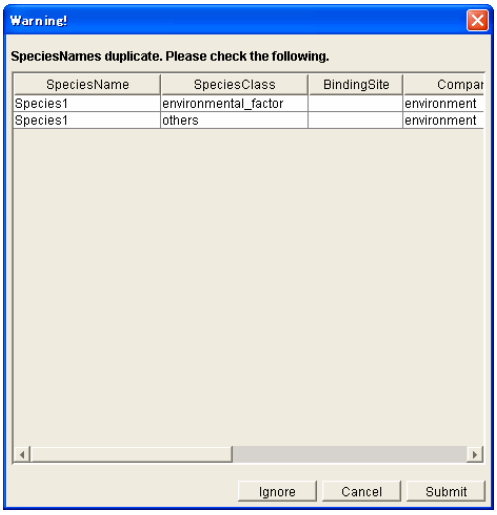
Start the OpenDialog box.
Loading an Existing Network Data in the dialog box. (4-3)

11-1-3 Save

Save the network data created and edited by NetworkConstructor, DateEditor, WhiteBoxTreeWindow, or FrameworkEditor. If the network is newly created, it will be always saved as "SaveAs."

The system alerts when the Species with the same name or different Compartments exist in a Compartment or when a Transport exits in a Compartment.

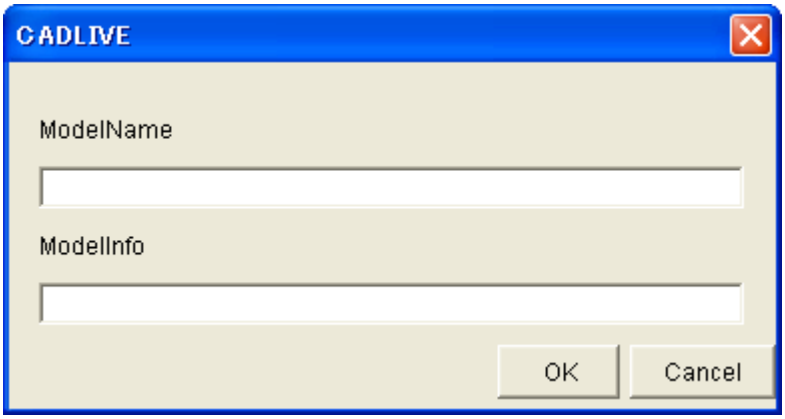
The system alerts when a Reaction has the wrong Layer. The errors involving a Layer are as follows:
* ReactionType is TRANSCRIPTION, TRNASLATION, or PROTEIN_SYNTHESIS, while Layer is not GENE.
* ReactionType is BINDING, ASSOCIATION, ELIMINATION, while LAYER is not PROTEIN.



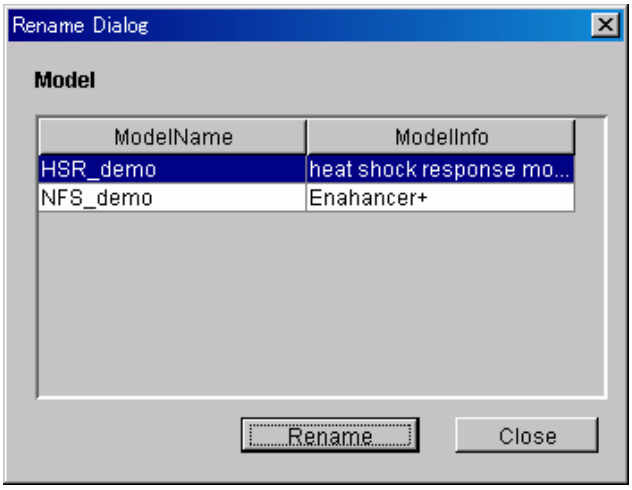
Clicking the Ignore button neglects the alert and saves the model, but an error may occur when the model is used by another system.
Clicking the Submit button improves the alerts involving SpeciesName or Layer and saves the model.
Clicking the Cancel button stops the Save process.

11-1-4 SaveAs

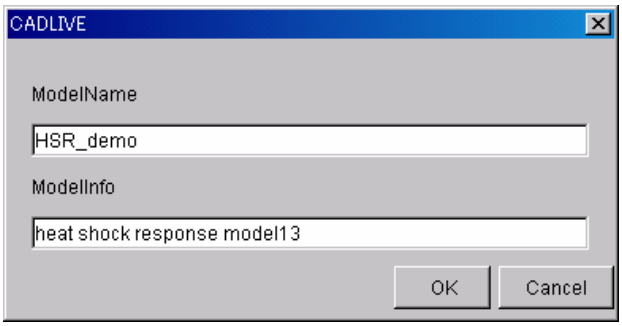
Network data is saved as ModelName.
The input content is ModelName and ModelInfo as follows.
This process checks Species or Reactions as well as Save.



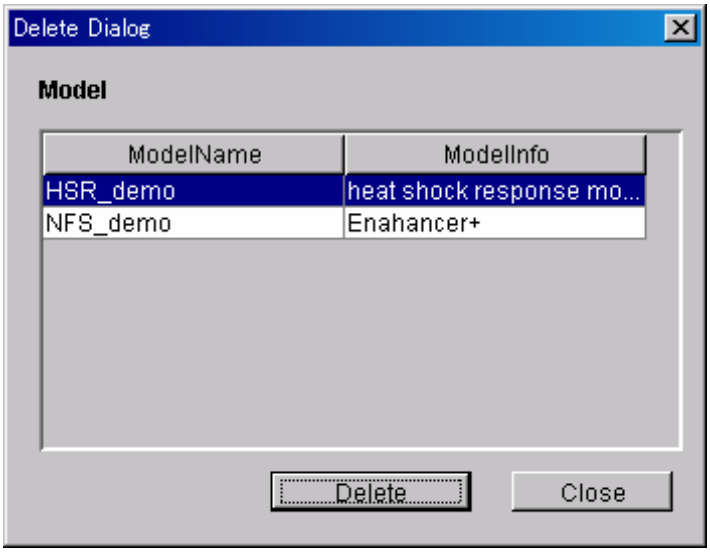
11-1-5 Rename



One displays the Rename Dialog, selects the model that one wants to rename from the spread sheet, and push the Rename button. One can rename ModelName and ModelInfo.

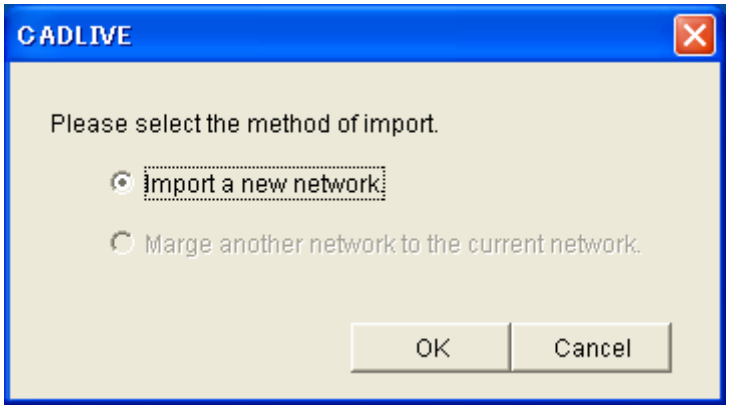


11-1-6 Delete



One displays the Delete Dialog, selects the model that one wants to delete from the spread sheet, and push the Delete button. The model is deleted.

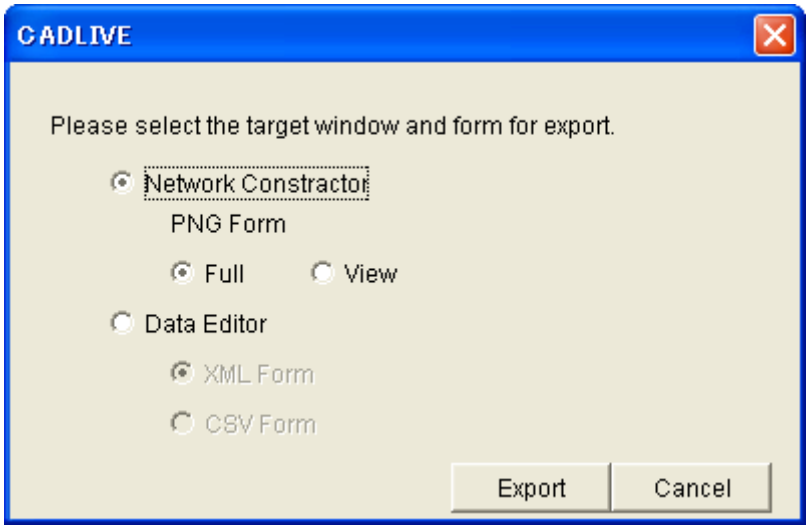
11-1-7 Import



Load an XML file that is created by another launched CADLIVE by selecting from the dialog.
>> Important a new network : a new XML file will be imported.
>> Marge another network to the current network : the XML file designated for the currently-edited network will be added.

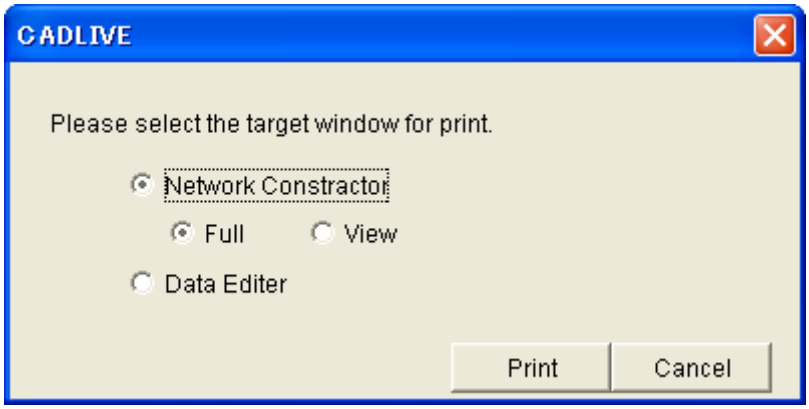
*The data that are created and edited by TextEditor are not allowed to import.

11-1-8 Export



The NetworkConstructor panel will be exported as a PNG image.
Full: The whole panel of NetworkConstructor will be exported as a PNG image.
View: The panel area of NetworkConstructor will be exported as a PNG image.
Species data and Reaction data of the network viewed in DataEditor will be exported as a specified format in specified place.
XML Form: will be saved in the XML format.
CSV Form: will be saved in the CSV format (comma-delimited text format)

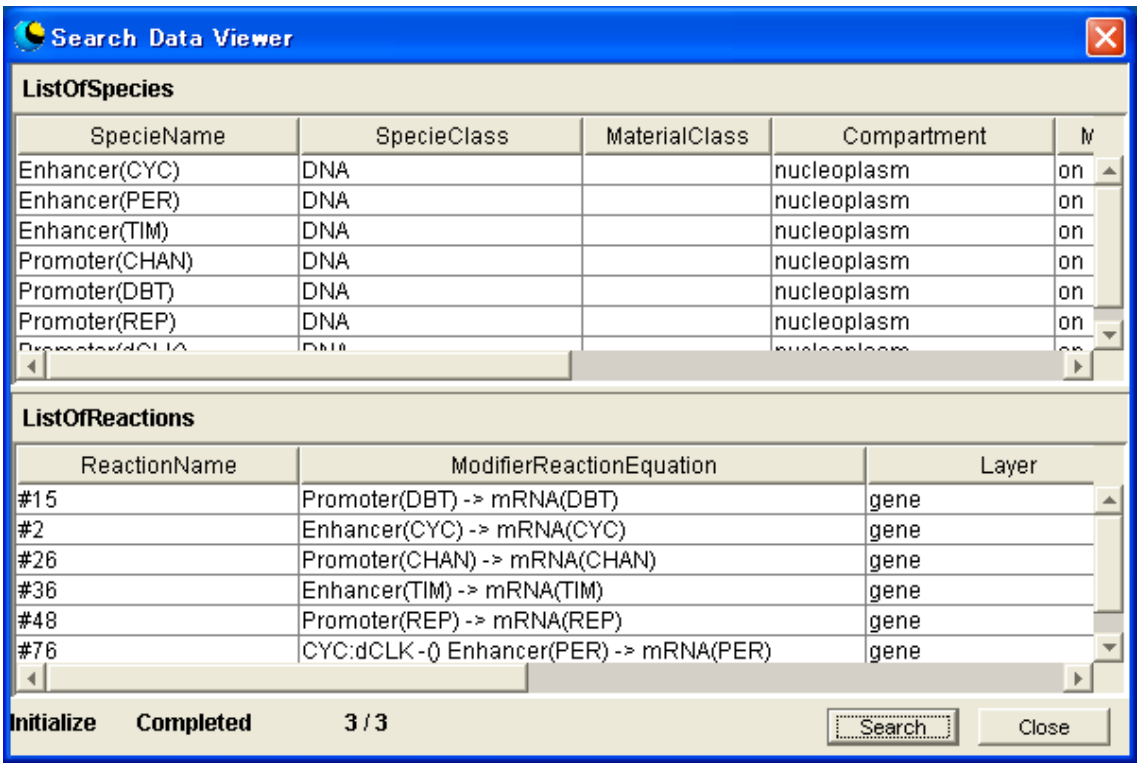
11-1-9 Print

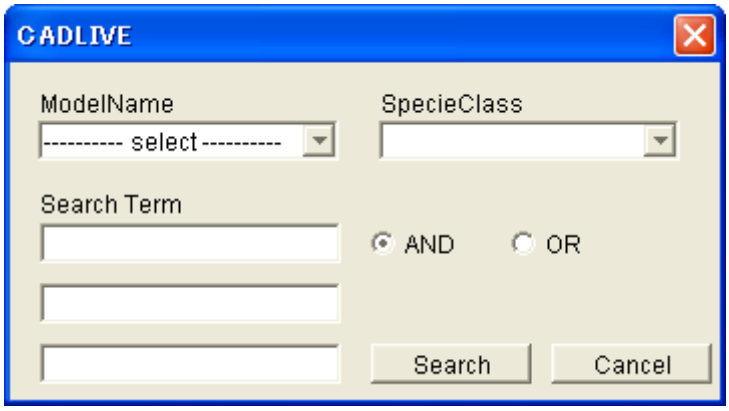


>> Printing the NetworkConstructor screen
Full: The whole panel area of NetworkConstructor will be printed on one page.
View: The panel viewing area of NetworkConstructor will be printed on one page.
>> Printing the DataEditor screen
The spreadsheet of DataEditor will be printed.

11-1-10 Search

Press the Search button on SearchDataEditor to display the Search Dialog box.





>> ModelName
Select a ModelName to search.

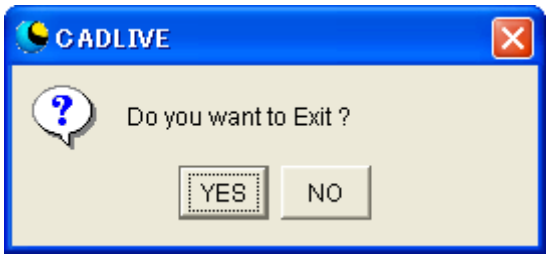
>> SpecieClass
Select the SpecieName of a species to search.

>> SearchTerm
Up to 3 SearchTerms can be input to search.

>> And/Or Radio Button
Select whether the character line input in "Search Term" will be searched on the "And" or "Or" condition.

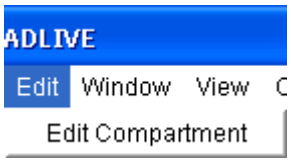
>> Search Button
Search the Reaction and Species applicable to the conditions input from XML networks and display them in spreadsheets of SearchedReaction and Searched Specie.

11-1-11 Exit

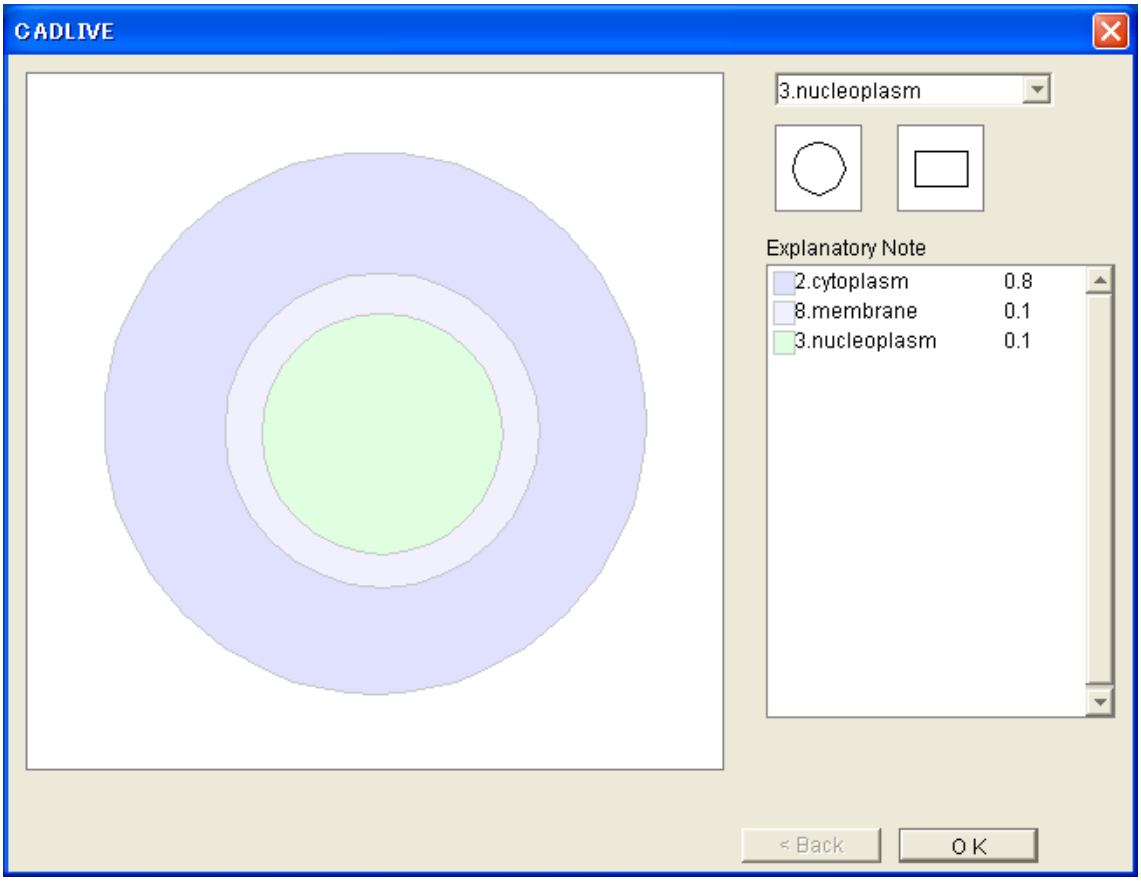


You are exiting CADLIVE SYSTEM

11-2 Edit Menu

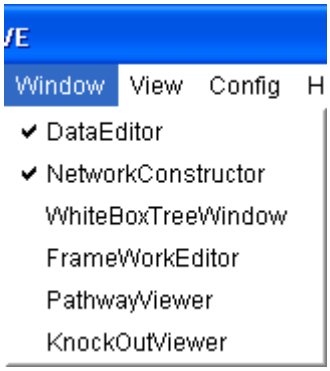


11-2-1 EditCompartment



The Window is displayed to reedit the Compartment.

11-3 Window Menu



11-3-1 DataEditor

When the DataEditor screen is visible, the menu is set to "Invisible." When it is invisible, it is set to "Visible." The check mark is displayed when the screen is visible.

11-3-2 NetworkConstructor

When the NetworkConstructor screen is visible, the menu is set to "Invisible." When it is invisible, it is set to "Visible." The check mark is displayed when the screen is visible.

11-3-3 WhiteBoxTreeWindow

When the WhiteBoxTreeWindow screen is visible, the menu is set to "Invisible." When it is invisible, it is set to "Visible." The check mark is displayed when the screen is visible.

11-3-4 FrameworkEditor

When the FrameworkEditor screen is visible, the menu is set to "Invisible." When it is invisible, it is set to "Visible." The check mark is displayed when the screen is visible.

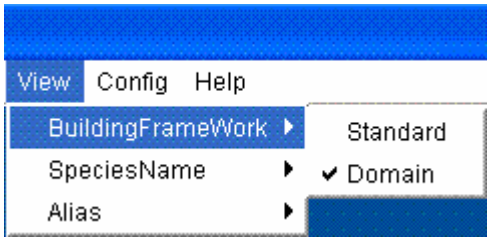
11-3-5 PathwayViewer

When the PathwayViewer screen is visible, the menu is set to "Invisible." When it is invisible, it is set to "Visible." The check mark is displayed when the screen is visible.

11-3-6 KnockOutViewer

When the KnockOutViewer screen is visible, the menu is set to "Invisible." When it is invisible, it is set to "Visible." The check mark is displayed when the screen is visible.

11-4 View Menu

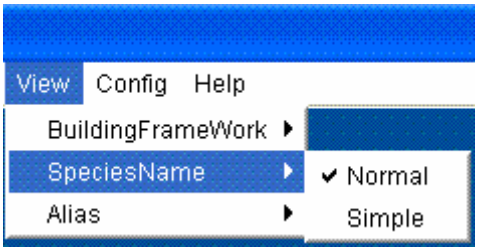


11-4-1 Standard

It is the mode that does not display any symbol peculiar to BuildingFramework (VirtualReaction, VirtualNode, Domain, InnerLink) on a screen.
Adding these symbols on NetworkConstructor changes to the Domain mode automatically.

11-4-2 Domain

All the Symbols are displayed.

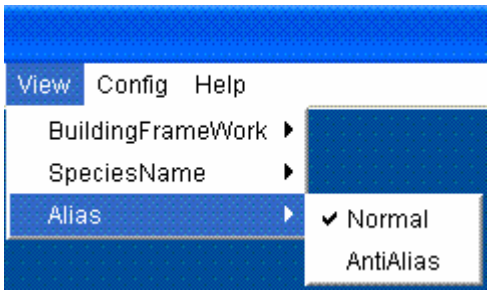


11-4-3 Normal

Ordinary SpeciesNames of Complex and Modified are displayed.

11-4-4 Simple

Abbreviate SpeciesNames of Complex and Modified are displayed.



11-4-5 Normal

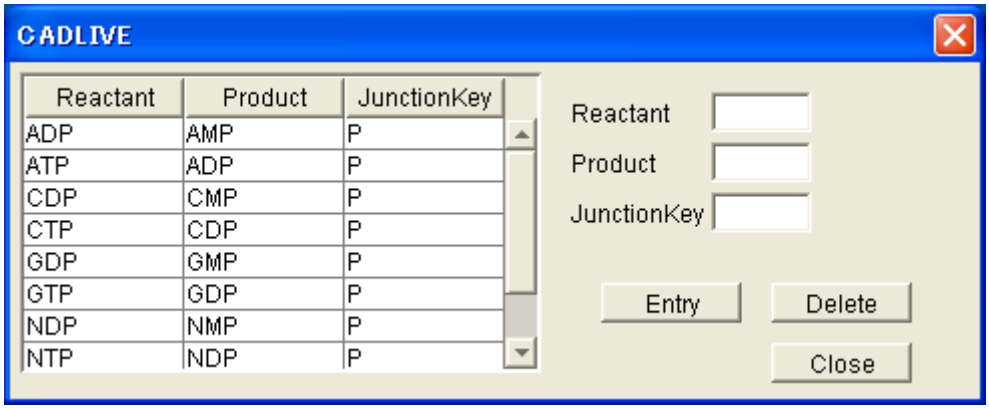
An image is displayed in an ordinary manner.

11-4-6 AntiAilas

AntiAlias displays a fine image.

11-5 Config Menu

11-5-1 SmallMolecule

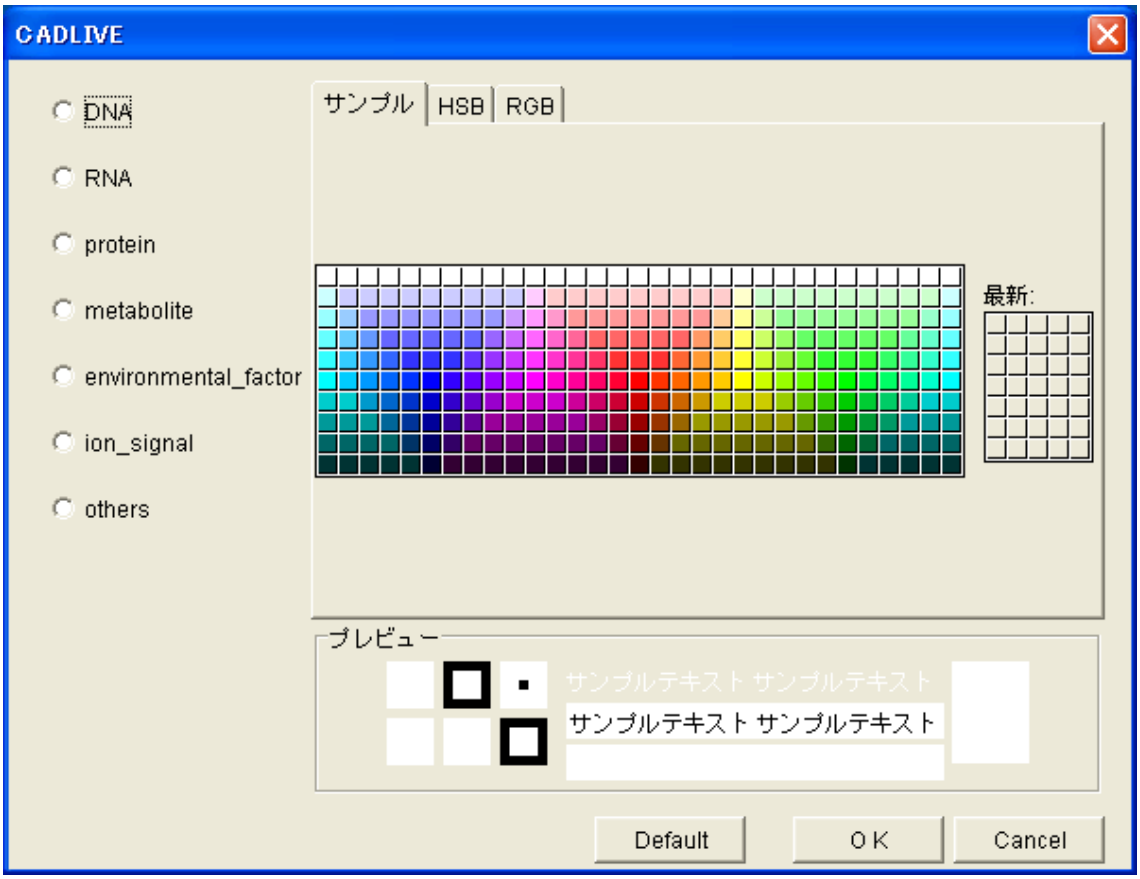


Configure Specie and JunctionKey, which are viewed when SmallMoleculeOption is added to the homo_association_wih_stoichimetric_change reaction.

>> Configuration
Input a character line in Reactant, Product, and JunctionKey, and press the Entry button.

>> Deletion
Select the Species and JunctionKey, press the Delete button.

11-5-2 SymbolColor



The viewing color of Species can be changed.

>> Configuration
After selecting the Species to configure on the left, select the color from the right and define it by pressing OK.
A plural number of Species can be configured simultaneously.
To set color as the initial color, press the Default button after selecting the Species on the left.

11-6 Help Menu

11-6-1 About CADLIVE

The version information of CADLIVE is displayed.