

# Systrip User Manual

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## Chapter 1

# Introduction

With the development of high throughput methods in biology, efficient visualization tools are more and more required. In particular it helps in understanding biological shifts induced on an organism by environmental stresses. In that case the data generated covers a wide range of biological processes which can be gathered into a single network. This network generally contains hundreds of elements and, prior to any in depth analysis, biologists are used to reduce the scope of their studies by selecting a few relevant sub-networks. The visual analytic process thus follows a top down approach consisting in filtering out steady part of the network. To help users in this visual mining we propose a flexible environment called Systrip.

Systrip is a perspective dedicated to biological network analysis and takes full advantage of the Tulip library and plug-in system. More than simply using Tulip library, Systrip adds a network manipulation layer on top of it. Such architecture aims at encapsulating both of graph manipulation and user interaction libraries. Relying on a graph structure gives to Systrip a great flexibility allowing to support both relational and multi-dimensional data. It also simplifies future integration of different biological networks (e.g. gene regulatory network or protein-protein interaction network).

This document describes Systrip features, as Systrip is based on the Tulip library you can find more detailed information on Tulip documentation <sup>1</sup>.

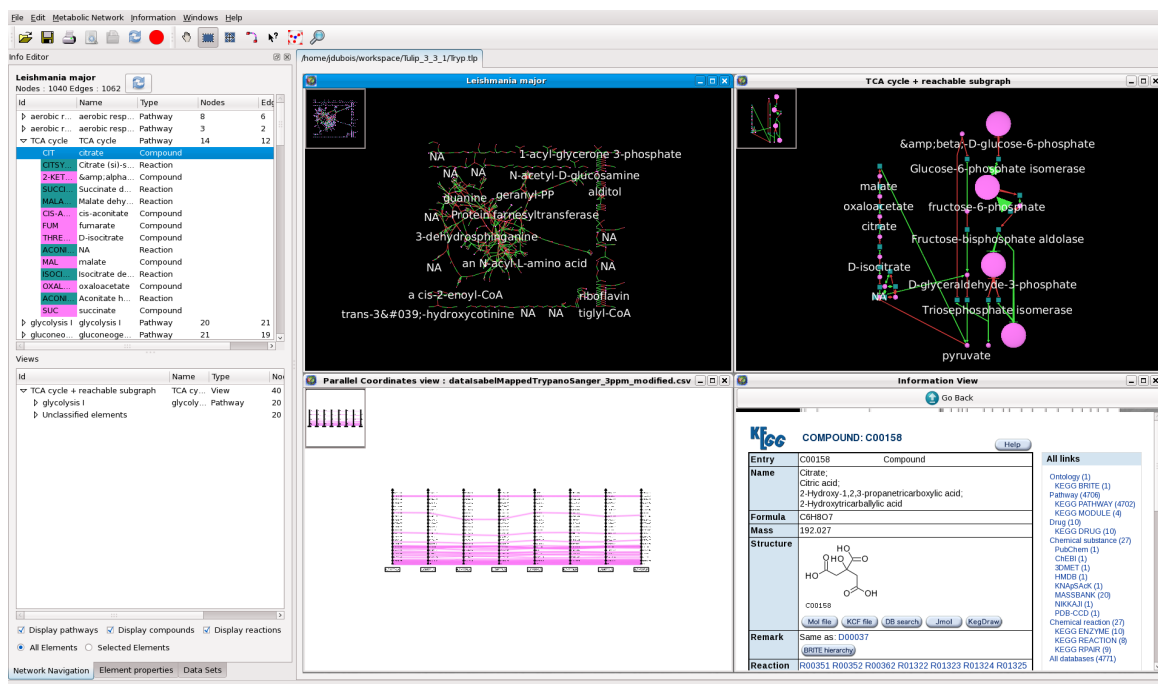


Figure 1.1: Systrip main view

<sup>1</sup> See [Tulip documentation web page](#)

## Chapter 2

# Graphic Interface

This chapter describes all the Systrip perspective user interface. The next picture shows the main organization of the Systrip interface.

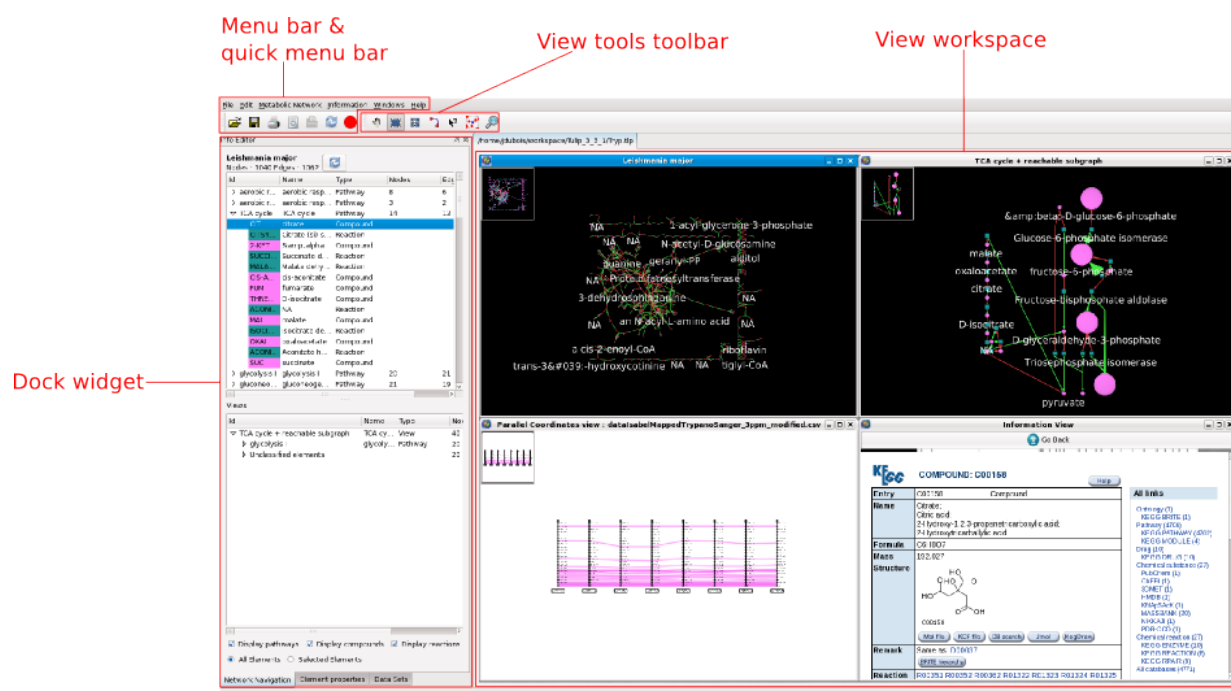


Figure 2.1: Decomposition of the Systrip graphical user interface.

Each part corresponds to a section.

## 2.1 Menu bar and menu tool bar

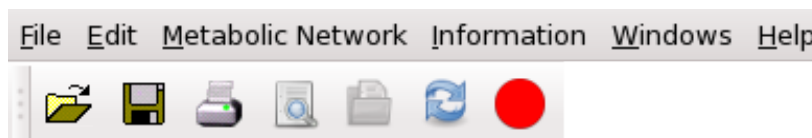


Figure 2.2: Menu bar and menu tool bar.

### 2.1.1 Menu bar

- **File** : this menu is used for usual file operations :
  - **New ( `Ctrl+N` )** : create a new Systrip perspective. Multiple perspective can be opened at the same time.
  - **Open ( `Ctrl+O` )** : open a saved Systrip perspective.
  - **Save ( `Ctrl+S` )** : save the current perspective. If there is an older one save overwrites with new data.
  - **Save As ( `Ctrl+Shift+S` )** : save the current state in a new file.
  - **Print ( `Ctrl+P` )**
  - **Exit ( `Ctrl+Q` )**
  - **Import** : this sub-menu is populated by import plug-ins. You don't need to use this menu for Systrip.
  - **Export** : this sub-menu is populated by export plug-ins allowing to save a tulip graph accordingly to a specified format. By default Tulip is able to export in GML and TLP formats. You don't need to use this menu for Systrip.
- **Edit**
  - **Clear selection** : deselect all selected elements.
  - **Search in** : this sub-menu allows to search elements in the graph.
    - \* **All elements ( `Ctrl+F` )** : search for elements in the full graph.
    - \* **Compounds** : search for elements in the compounds.
    - \* **Reactions** : search for elements in the reactions.
    - \* **Pathways** : search for elements in the pathways.
  - **Preferences** : displays the preferences dialog.
  - **Advanced mode** : check button to switch from simple to advanced user interface.
- **Metabolic network** : contains all the actions related to the metabolic network.
  - **Import network** : loads a metabolic network in Systrip from an sbml file. Only one network can be loaded, after the button is disabled.
  - **Redraw current view ( `Ctrl+R` )** : erase the old layout perform a new one for the selected widget.
  - **Redraw network** : redraw the root network layout. If network widget does not exist create new one.
  - **Restore default parameters** : restore the visual parameters defined in the preferences dialog for the metabolic network and all its views.
  - **Analysis** : from this menu you can apply analysis algorithms on the selected view. The algorithms present in this menu are specially designed and configured to work with metabolic networks. They are separated in distinct types.
    - \* **Graph measure** : this sub-menu is populated by 'metric' algorithms. These algorithms allow to compute and assigne a value to the 'viewMetric' property of graph elements. For example, when running the 'Degree' algorithm, the degree (the number of a node neighbors) of each node is computed and stored in the 'viewMetric' property.
    - \* **Biological selection** : this sub-menu is populated by 'selection' algorithms. These algorithms allow to select nodes and or edges satisfying some criteria.







- **Algorithms** : only visible in advanced graphical mode. This menu apply algorithms on the selected network view or on the full network if no one is selected. It is divided in several parts to make a difference between the kind of algorithms you can apply. For more information please visit the Tulip documentation <sup>1</sup> on algorithms(section 3.2) and graph properties(section 3.3).
  - **Selection** : this sub-menu is populated by 'selection' algorithms. These algorithms allows to select nodes and or edges satisfying some criteria. For example the 'Loop Selection' algorithm detects all edges for which the starting and ending nodes are the same.
  - **Color** : this sub-menu is populated by 'color' algorithms. These kind of algorithm computes the color of the graph elements. A default one, 'Metric Mapping', is provided; it allows to color all graph elements according to a metric property.
  - **Measure** : this sub-menu is populated by 'metric' algorithms. These algorithms allow to compute and assign a value to the 'viewMetric' property of graph elements. For example, when running the 'Degree' algorithm, the degree (the number of its neighbors) is computed and assigned to each graph node 'viewMetric' property.
  - **Layout** : this sub-menu is populated by 'layout' algorithms which allow to display graphs using different types of drawings. For example, the 'Circular' algorithm places all nodes of a graph along a circle.
  - **Size** : this sub-menu is populated by 'size' algorithms which allow to compute the size of the graph elements.
  - **General** : this sub-menu is populated by more general algorithms for computing properties, subgraphs, quotient graphs, groups... For example the 'Equal Value' algorithm create subgraphs for which the included elements have the same value for a choosed 'metric' property.
- **Information** : this menu contains all the external database operations.
  - **Display information for selected nodes** : query databases for each selected node.
  - **Clean information view** : clean the information view, this option does not erase the downloaded data.
  - **Clear collected information** : clean the information view and erase the downloaded data.
  - **Edit database priority** : edit the query order for external databases.
  - **Database properties** : this menu allows user to edit parameters for each external databases.
- **Windows** : this menu contains two options for the management of the views in the workspace.
  - **Cascade** : Arranges all the child windows in a cascade pattern.
  - **Tile** : Arranges all child windows in a tile pattern.
- **Help** : in this menu, you can find information about the software and plug-ins management options. See the Tulip documentation <sup>1</sup> for more information on it.




### 2.1.2 Menu tool bar

This tool bar contains 7 shortcut :



Figure 2.3: Menu tool bar.

- **Open ( **Ctrl+O** )** : open a previously saved Systrip state. 
- **Save ( **Ctrl+S** )** : save the current state in a Tulip graph. If there is an older one save overwrites with new data. 
- **Print ( **Ctrl+P** )** 
- **Search in all elements ( **Ctrl+F** )** : search for elements in the full graph. 

- `Import network` : load a metabolic network in Systrip from an sbml file. Only one network can be loaded, when it's done the button is disabled. 
- `Redraw current view ( Ctrl+R )` : if a metabolic network view is selected in the view workspace erase the old layout perform a new one for this view. 
- `Record selected view` : create a video from the activated view. If the selected is not compatible with video recording, this icon is disabled. 

## 2.2 Dock widget

This is the main widget for interact with data loaded in Systrip. It contains data manipulation widgets like metabolic network widget or data sets widget. Here is the list of the widget you can find in the dock widget :

- `Network navigation` : metabolic network navigation and manipulation.
- `Element properties` : properties visualization for selected nodes.
- `Data sets` : data sets management widget.
- `Advanced options` : only visible in advanced mode. Contain the view, interactors and video configuration widgets.

To switch between the different widgets just click on the corresponding tab at the bottom of the dock widget.

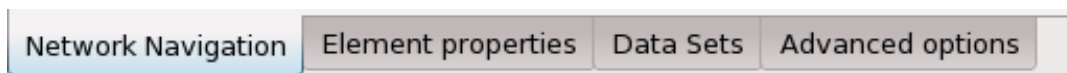


Figure 2.4: Dock widget tabs.

### 2.2.1 Metabolic network navigation widget

The metabolic network is the set of biochemical reactions that occur in a living system. Each reaction transforms a set of molecules (or metabolites) called substrates into other molecules called products. In Systrip reactions and molecules are represented by nodes, a reaction is linked to a molecule only if this reaction consumes or products this molecule. Networks can be divided in smaller parts called metabolic pathways. Like in the network, pathways are composed of reactions and substrates. Different pathways can have overlapping sets of reactions and pathways but each pathway must have a unique name.

Another important feature of Systrip is the capability to create a copy of the full network or of a sub-part of it and work with them without altering the original data. These copies are called *metabolic views* . When designing Systrip tool, we tried to find an intuitive data and views management and used an analogy to book reading : when reading a book, one usually does not write in it but prefer to use a sheet of paper or a draft. This helps to summarize the section(s) one has read or to "play" with ones ideas in order to find new insights without damaging the book itself. In Systrip, the user can therefore use one or several drafts corresponding in our case to views on sub-networks of interest.

The link between each metabolic view and its network is one-way. Modifications in a metabolic view don't affect network but conversely modifying network elements or pathways will affect each view containing these pathways or elements. This relation allows to work with metabolic views without altering original and to easily revert modifications.

Both full network and metabolic views can be draw in Systrip, each with a specific representation. There are several drawings methods in Systrip (for more information about network and metabolic views drawing see Section 3.1 ).

### 2.2.1.1 Metabolic network widget

This widget is used to visualize and edit metabolic network. The next picture describes its interface.

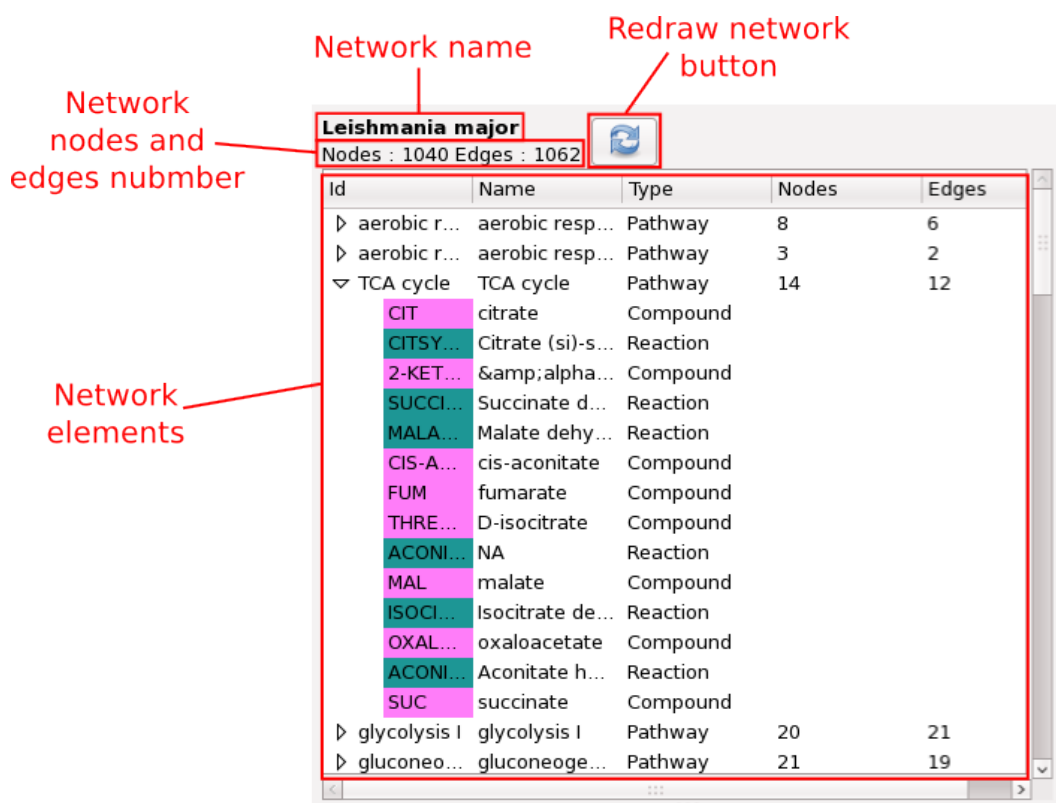


Figure 2.5: Metabolic network widget interface description.

Networks are represented as a tree : pathways are inner nodes containing a leaf node for each reaction and compound. The specific node called `Unclassified elements` regroup all the elements that don't belong to any pathway.

Each node has fields to add information on the element it represents. Here is the list of the fields with a description:

- **Id** : the id of the element. For pathways Id and Name fields are the same.
- **Name** : the name of the element.
- **Type** : this field give the type of the element. There is three types of items : pathway, compound and reaction.
- **Nodes** : filled only for pathway items. Give the number of nodes for the pathway. If there is selected nodes in the pathway their number is append between brackets.
- **Edges** : filled only for pathway items. Give the number of edges for the pathway. If there is selected edges in the pathway their number is append between brackets.

User can create pathways from the contextual menu. Each new pathway must have unique name. Once created user can fill it with existing elements. To add an element just drag and drop it on the pathway to add it. Actually user can only drag and drop compounds or reactions.

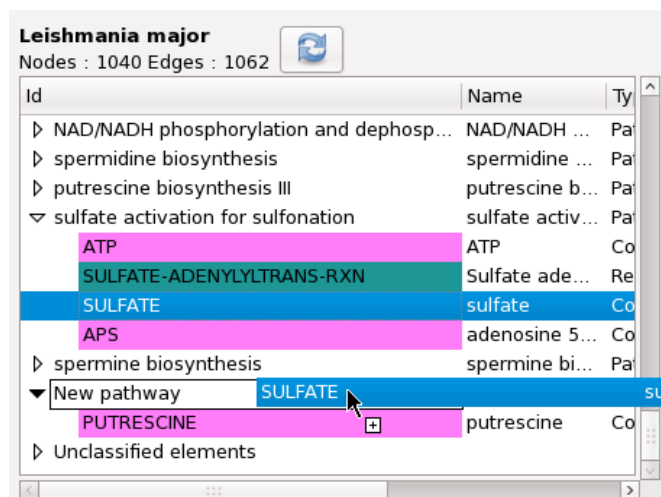


Figure 2.6: Add an element by drag and drop.

To delete elements user can either use the contextual menu or press the `Del` or `Backspace` key. Removing an element in a pathway subtree removes it from the pathway. When an element no longer belongs to any pathway, it will be displayed in the `Unclassified elements` inner node. Deleting an element from the `Unclassified elements` inner node removes it definitely.

#### 2.2.1.1.1 Contextual menu

By right clicking on this widget user can show a contextual menu. This menu differs in function of the selected element type.

- `Rename` : only visible when clicking on pathway item. Rename the selected pathway.
- `Show properties` : display the available information on the selected element (pathway, compounds or reaction).
- `Select / Deselect` : select all unselected or partially selected elements and unselect others.
- `Delete` : delete the selected element. If it's a pathway these internal elements will not be erased.
- `Create new pathway` : create an empty pathway.
- `Create new pathway from selection` : create a new pathway with current selection as base elements.

#### 2.2.1.2 Metabolic views widget

This widget allow user to create, delete and edit metabolic views. This widget is similar to the network widget presented before. Each metabolic view is represented in the tree widget by inner nodes regrouping its pathways, reactions and compounds nodes.

There are two ways to create a new metabolic view. The first by using contextual menu on the metabolic view management widget. Select the `Create new view` or `Create new view from selection` menu (see Section 2.2.1.2.1).

The second solution is to drag and drop elements from metabolic network widget. There is multiple drag and drop possibilities from the network widget. First you can simply drag pathway or element from the network widget to the metabolic view widget (be sure to don't drop element on an existing view or you will modify it). This solution simply creates a new view with the dragged element as base element.

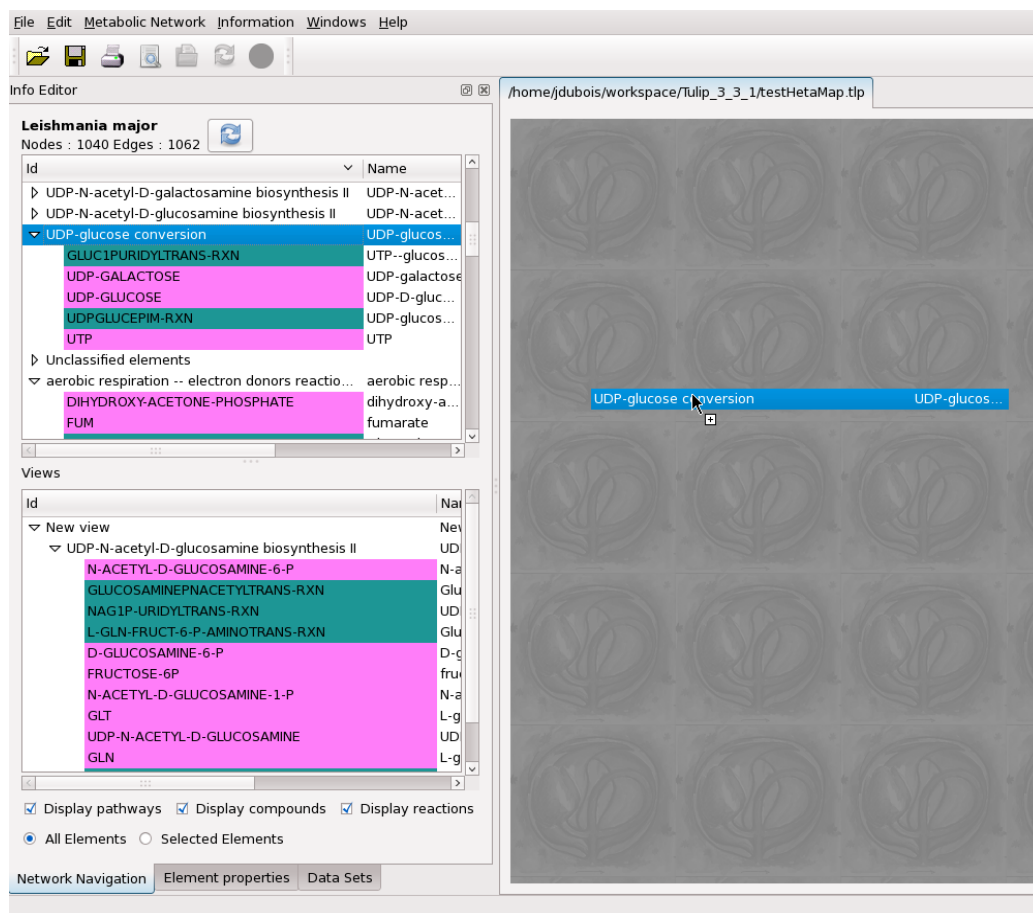


Figure 2.7: Creation of metabolic view by dragging a pathway on view workspace.

You can also drop the selected element on the view workspace, this solution create a new view and draw them immediately.

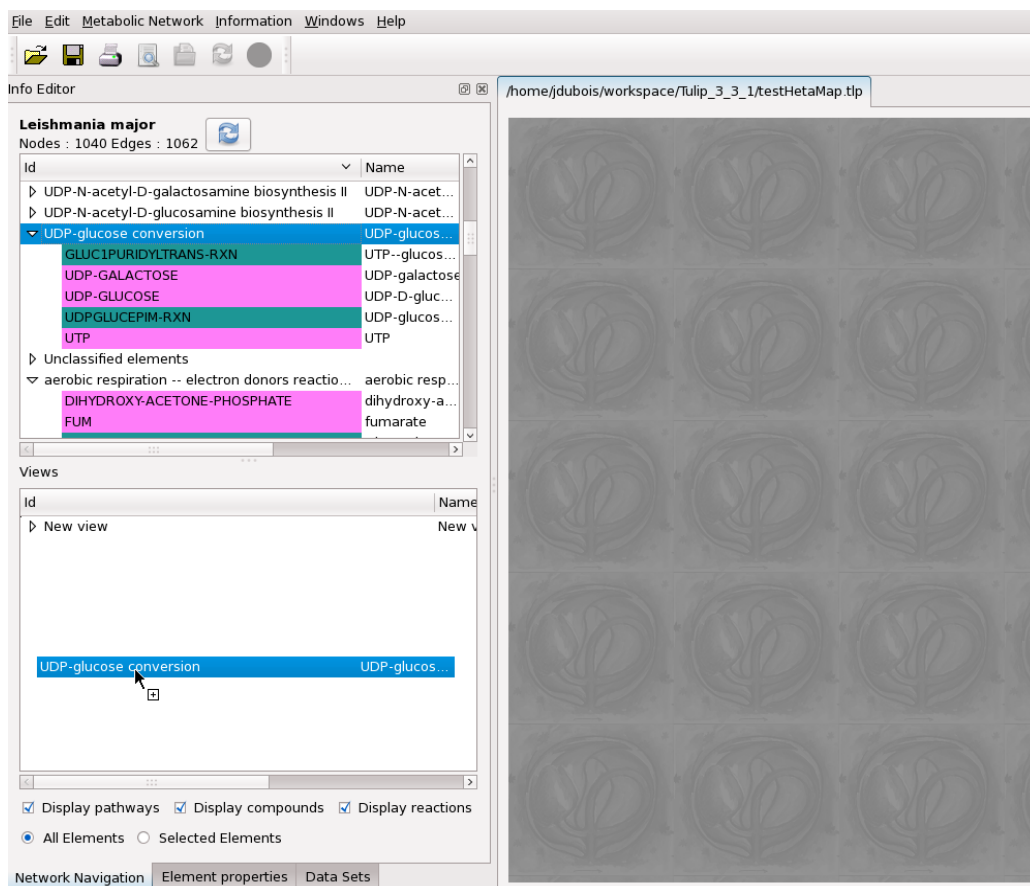


Figure 2.8: Creation of metabolic view by dragging a pathway on metabolic view widget.

For the both methods when creating a new metabolic view a dialog appears to query its name. If you enter an existing name an error message will appear and the creation will be canceled.

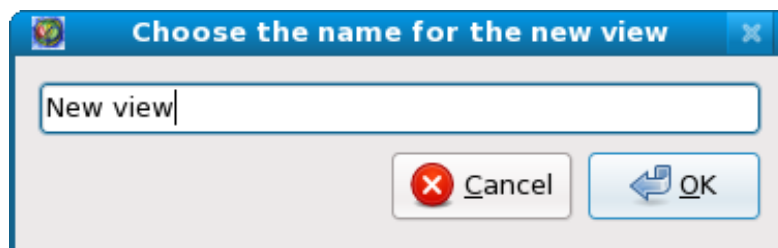


Figure 2.9: Metabolic view name selection dialog.

To add element in an existing view just drag and drop it on the metabolic view name. If the element don't exists in the metabolic view it will be automatically added.

To delete a view user can either use the contextual menu or press the `Del` or `Backspace` key. When destructing a metabolic network view all it's modification are lost and all the widget related to it's view are closed.

User can focus on a specific metabolic view by double clicking on it in the metabolic view widget. A small icon appear next



to the selected metabolic view : Once selected the network color is updated to highlight the selected network view. To deselect a metabolic view double click on it.

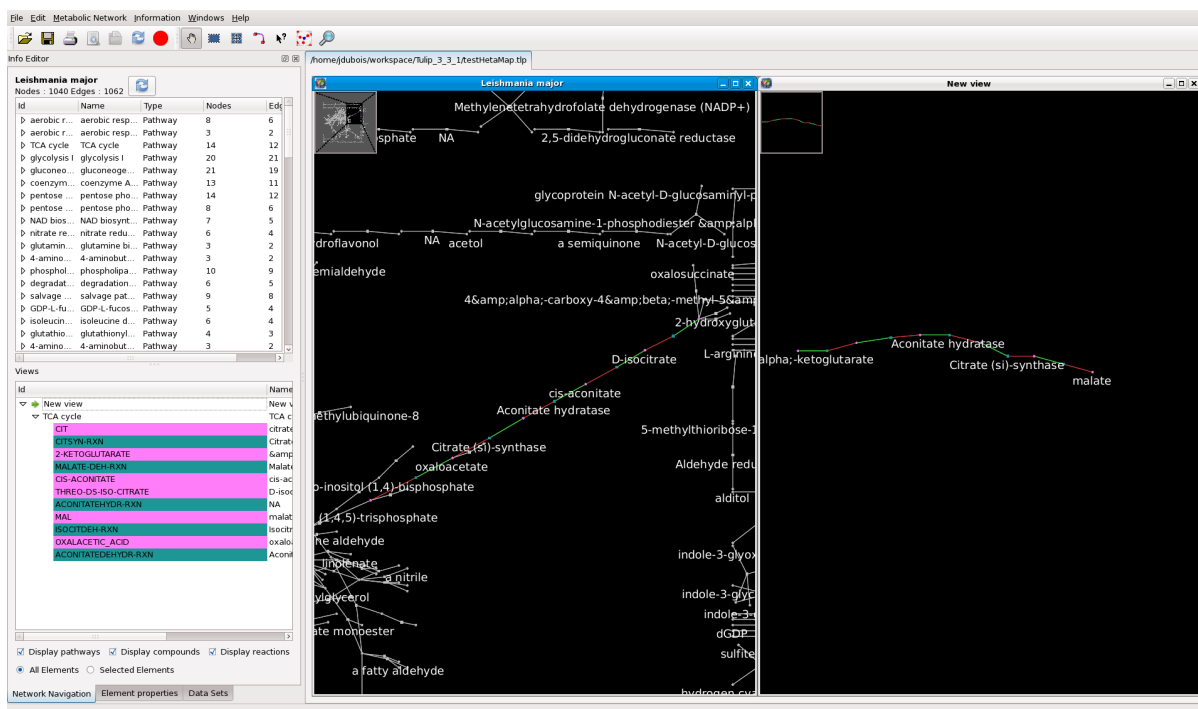


Figure 2.10: Metabolic view selection example.

### 2.2.1.2.1 Contextual menu

By right clicking on this widget user can show a contextual menu. This menu differs in function of the selected element type.

- **Rename** : only visible when clicking on pathway item, rename the selected pathway.
- **Show properties** : display the available information on the selected element (pathway, compounds or reaction).
- **Select / Deselect** : select all unselected or partially selected elements and unselect others.
- **Delete** : delete the selected element from the network. If the deleted element is an internal element, it will be definitely lost. If the element is a pathway these internal elements will be not erased.
- **Create new pathway** : (only visible when a view is selected) create a new pathway with no elements.
- **Create new pathway from selection** : (only visible when a view is selected) create a new pathway with current selection as base elements.
- **Create new view** : create an empty new view.
- **Create new view from selection** : create a new view with current selection as base elements.

### 2.2.1.3 Tree widget elements control widget.

This widget controls the display of tree widget elements for both metabolic network and metabolic network view widgets. It allows to display elements according to their types (compounds, reactions, pathways) and their states (selected or not).

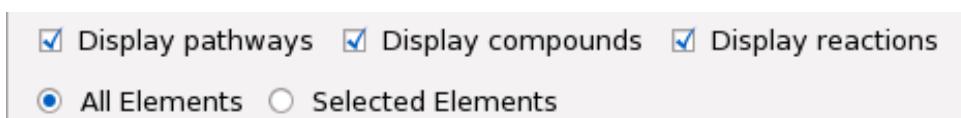


Figure 2.11: Elements display control buttons.

The first row of buttons is the type filter. It allow to choose which kind of elements to display.

- `Display pathways` : if checked display the pathways elements. If unchecked all the elements of the network of the view are displayed in the root elements.
- `Display compounds` : display the compounds elements.
- `Display reactions` : display the reactions elements.

The second buttons row allows to filter elements according to their selection state. User can display all the elements or only the selected elements. When displaying selected elements only selected reactions and compounds are displayed, for pathway items only pathways containing selected compounds or reactions are displayed.

### 2.2.2 Elements properties widget

This widget displays graph properties for an element. When a user query information for a node this widget is automatically shown and a selection of properties are display with their values. Only one node can be displayed at a time. The element type and its name is displayed at the top of the widget. User cannot change properties values.

| Reaction : Malate dehydrogenase |  |
|---------------------------------|--|
| Id                              | Property   |
| id                              | MALATE-DEH-RXN   |
| name                            | Malate dehydrogenase                                     |
| subSystem                       | gluconeogenesis<br>aspartate degradation II<br>TCA cycle |
| reversible                      | true   |
| listOfReactants                 | malate   |
| listOfProducts                  | oxaloacetate   |

Figure 2.12: Default properties for the Malate dehydrogenase reaction.

You can set the properties list to display for compounds or reactions in the `Information table` tab of the preferences dialog (see preferences dialog section Section 2.4 )

### 2.2.3 Data sets widget

Systrip allows to import and visualize time series expression data on metabolic network nodes.

From this widget user can perform all the possible operations on data sets. It can be divided in two separate widgets with distinct functionality : `Data sets management widget` and `Data set animation widget`.



Data sets  
management widget

Data set animation  
widget

The screenshot shows the 'Info Editor' window with two main sections highlighted by red boxes and labels. The top section, 'Available Data Sets', contains a table with columns 'Id' and 'Name'. The first row is highlighted in blue and contains a folder icon, a green icon, and the filename 'datalsabelMappedTrypanoSanger\_3ppm\_modified.csv'. Below this, a list of chemical names is displayed, with the first few rows highlighted in pink. The bottom section, 'Animation controller', shows 'Current Properties : II\_GMS224\_A' and a large empty rectangular area. Below this area are navigation buttons: a double left arrow, a single right arrow, a square, and a double right arrow. At the bottom of the window are three tabs: 'Network Navigation', 'Element properties', and 'Data Sets'.

| Id  | Name |
|---|------|
| datalsabelMappedTrypanoSanger_3ppm_modified.csv |      |
| GAP   | D-g  |
| NN-DIMETHYLANILINE                              | N,N  |
| 3-HYDROXY-L-KYNURENINE                          | 3-h  |
| L-ALPHA-ALANINE                                 | L-a  |
| MET   | L-n  |
| LEU   | L-le |
| ANTHRANILATE                                    | ant  |
| GLT   | L-g  |
| PHOSPHORYL-ETHANOLAMINE                         | pho  |
| GLC-1-P   | &a   |
| GLYCEROL-3P                                     | sn-  |
| D-GLUCOSAMINE-6-P                               | D-g  |
| FRUCTOSE-6P                                     | fru  |
| DIHYDROXY-ACETONE-PHOSPHATE                     | dih  |
| HOMO-SER  | hor  |
| XANTHOSINE                                      | xar  |

Import new data set

Current dataset properties

Animation controller

Current Properties : II\_GMS224\_A

Reset View

Network Navigation | Element properties | Data Sets

### 2.2.3.1 Data sets management widget

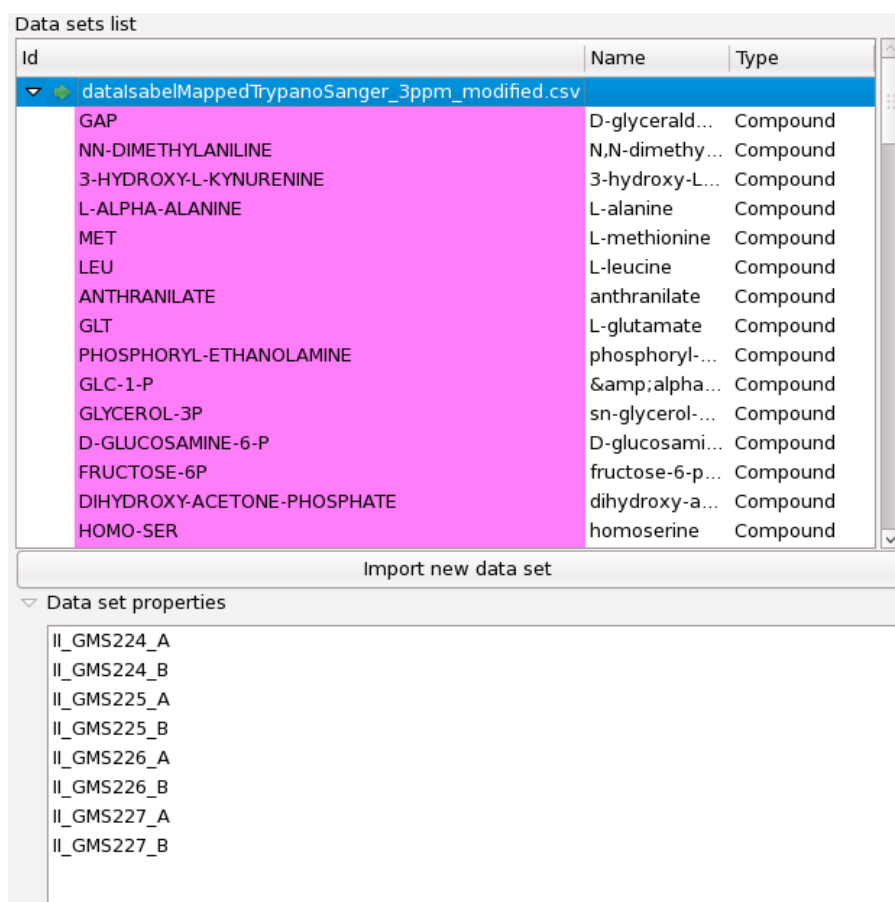


Figure 2.13: Data sets management widget.

This widget is responsible of all the data set management operations. The `Data sets list` widget is the main component it displays the list of loaded data sets. User can expand each data set to show their elements. The `Data set properties` widget is used to list the properties of each data sets.

By double clicking on a data set in the list the user can animate them. This action allow to use animation on data set see Section 2.2.3.2 for more information on data set animation. Only one data set can be animated at the same time.

#### 2.2.3.1.1 Contextual menu

By a right mouse button press on `Data sets list` widget user can call the contextual menu. It can be different if user call it on an element or not. If an element is under the cursor when user right click element's special options are added to the menu.

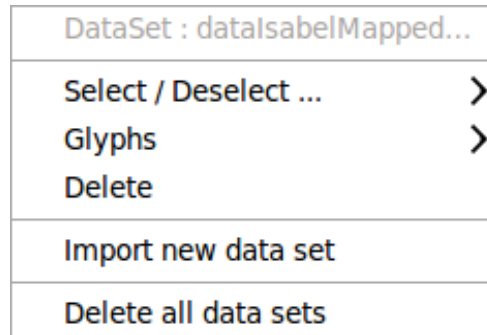


Figure 2.14: Data set widget contextual menu.

- `Select / Deselect ...` : only visible when clicking on a data set element
  - `All elements` : if all the elements of the data set are unselected or partially selected, select them else unselect them.
  - `Most changing elements` : select or unselect only the most changing elements of the data set (elements with the greatest variation between each time). When clicking on it a dialog is shown querying the number of elements to select. If all these elements are unselected or partially selected select them else unselect them.
- `Augmented display` : (only visible when a data set is selected) the augmented display selection menu is used to apply or remove specific information over each element of a data set. See the augmented display section (Section 2.4) for more information on elements you can display over data sets nodes.
- `Import new data set` : import a new data set. If you want more details on data sets importation see Section 2.2.3.1.3 .
- `Delete` : delete the selected element data set or node. If the element is a node remove it from the data set.
- `Delete all data sets` : remove all the data sets.

### 2.2.3.1.2 Augmented display

This widget allows user to display augmented information for the selected data set. Select the information you want to display and click on the apply button. To hide displayed information choose the `No display` value and click on apply.

Here is a list of the kind of information you can display over data set elements.

- `Display heat maps` : display the heat map information. Each time point is represented by a rectangle. The rectangle's colour depends on the value of the represented time point. The colours are computed this way : we divide the data set values interval in ten parts and we map a colour for each parts.

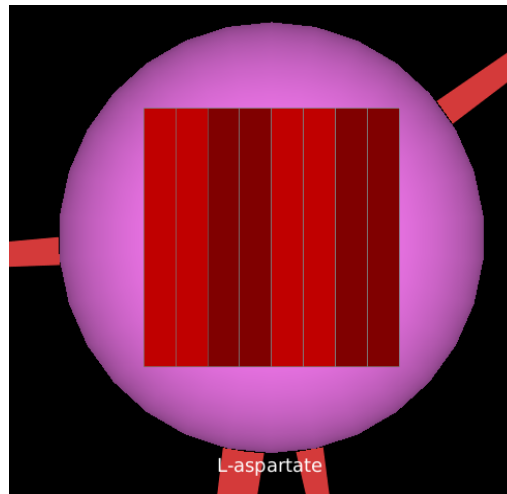


Figure 2.15: Heat map



Figure 2.16: Heat map colour mapping.

- **Curve** : build a curve with values of the node. The time series are mapped along the horizontal axis and values along the vertical axis.

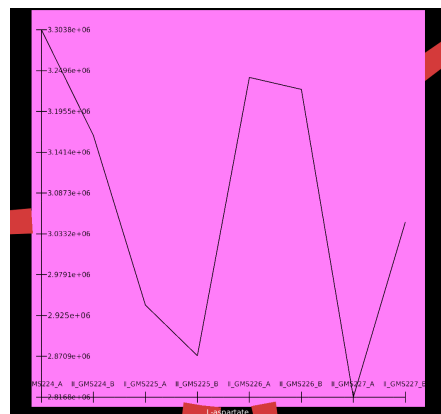


Figure 2.17: Curve sample.

### 2.2.3.1.3 Data sets importation

At this time data sets can be created only from CSV files. Values can be organized in row or column but the first value of the list must be the element id.

The next widget ( Figure 2.18 ) is used to turn CSV file into data set.

**Import data set**

**File parameters**

Csv file:

Separator:

☒ Use first row as property name

**Properties**

☒ ☒ ☒ ☒ ☒ ☒ ☒

**Preview**

|   | sbmlID   | II_GMS227_A | II_GMS227_B | II_GMS224_A | II_GMS224_B | II_GMS225_A | II_GMS225_B | II_GMS226_A | II_GMS226_B |
|---|----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 1 | UREA     | 188137      | 211619      | 333481      | 315928      | 234757      | 229110      | 244940      | 256897      |
| 2 | CPD-6082 | 21767157    | 25069216    | 26480666    | 24898391    | 24003818    | 24467654    | 27027978    | 24752181    |
| 3 | LACTALD  | 20284       | 21066       | 16396       | 12503       | 27345       | 23901       | 10389       | 11624       |
| 4 | ACETOL   | 20284       | 21066       | 16396       | 12503       | 27345       | 23901       | 10389       | 11624       |
| 5 | GLY      | 9502121     | 10220226    | 12170409    | 11265508    | 11182792    | 11281498    | 10972433    | 10996280    |

Figure 2.18: Data sets creation widget from CSV file.

Here is a description for each element of this widget :

- **Filename** : this field must contain the csv file to load.
- **Separator** : this field contains the separator of the CSV file.
- **Use first row (or column) as time series names** : if checked the first row (or column if data are organized in column) is treated as labels for loaded time series. If unchecked the time-series name are automatically generated.
- **Properties** : this list allows you to configure the properties you want to import. You can edit the property name or choose if you want to import the property by checking or unchecking the checkbox over the property name.
- **Preview** : this widget just gives a preview of the csv file. If a property is not imported it will appear in gray in this preview widget.

Once the widget fields are filled with the right values, click on the **Ok** button to launch the data set importation. Data sets name are generated from the name of the file loaded. If you try to load a file with the same name with an existing data set this dialog will appear.

A dataset with the same name already exist do you want to replace it?

- **Cancel** : cancel the import.
- **Rename** : change the name of the new data set and import them.
- **Replace** : delete the existing data set and import the new one.

### 2.2.3.2 Data set animation widget

This widget is responsible for data sets animation. User can animate nodes size from in function of the current time point value. Nodes are growing or shrinking in function of their data from the different time series.

#### 2.2.3.2.1 Animation properties widget

This widget controls all the animations parameters. Only visible in advanced mode it allows to configure the animation parameters like the time of animation or the mapping parameters.

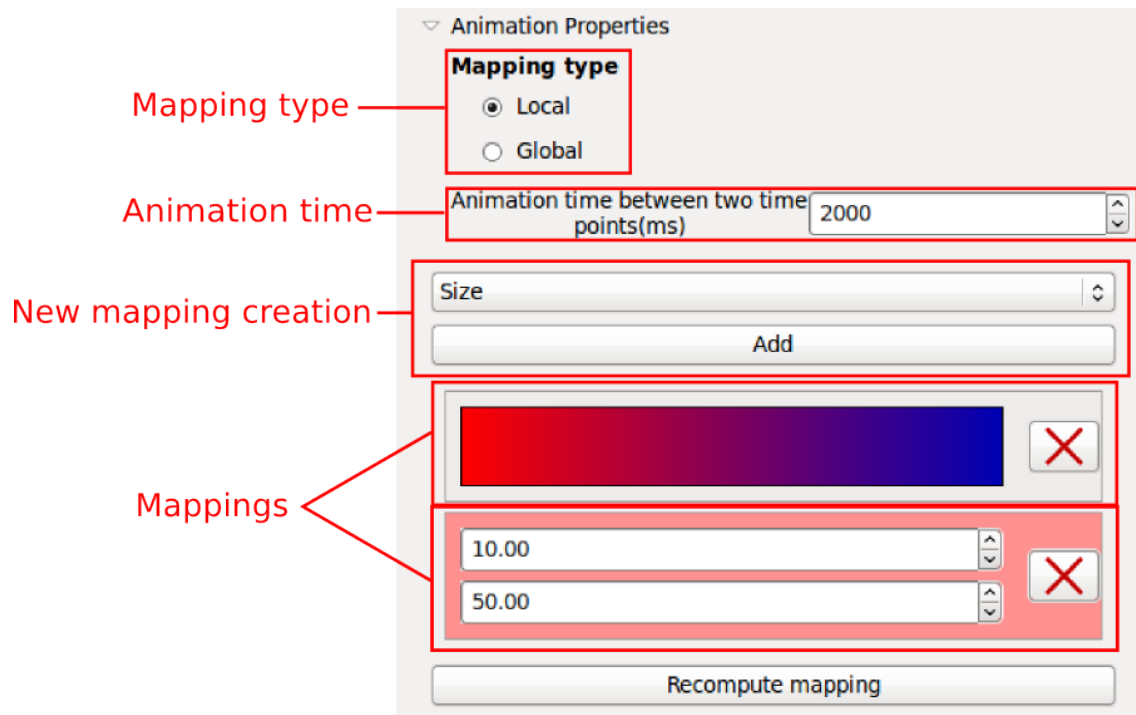


Figure 2.19: Animation properties widget.

- **Mapping type** : define if the mapping for a node is computed only from its own values ( `Local` ) or from all the values of the data set( `Global` ).
- **Animation time** : the animation time between two time points in millisecond.
- **New mapping creation** : use the combobox to select the kind of mapping element you want to add and click on the add button. There is two kind of mappings size and color mapping.
- **Mappings** : this is list of mapping elements. To delete a mapping element click on its red cross button. Each mapping can be edited. If the background of an element appears in red it means this element has changed and the whole mapping need to be recomputed to take in account modification.
- **Recompute mapping** : if a mapping is just created, edited or deleted mappings need to be recomputed to take modification in accounts. Click on this button to recompute mapping. If mapping don't need to be recomputed this button is disabled.

To validate modifications press the apply button.

### 2.2.3.2.2 Animation control widget

This widget controls the animation. User can start, stop or change the current time stamp from this widget.

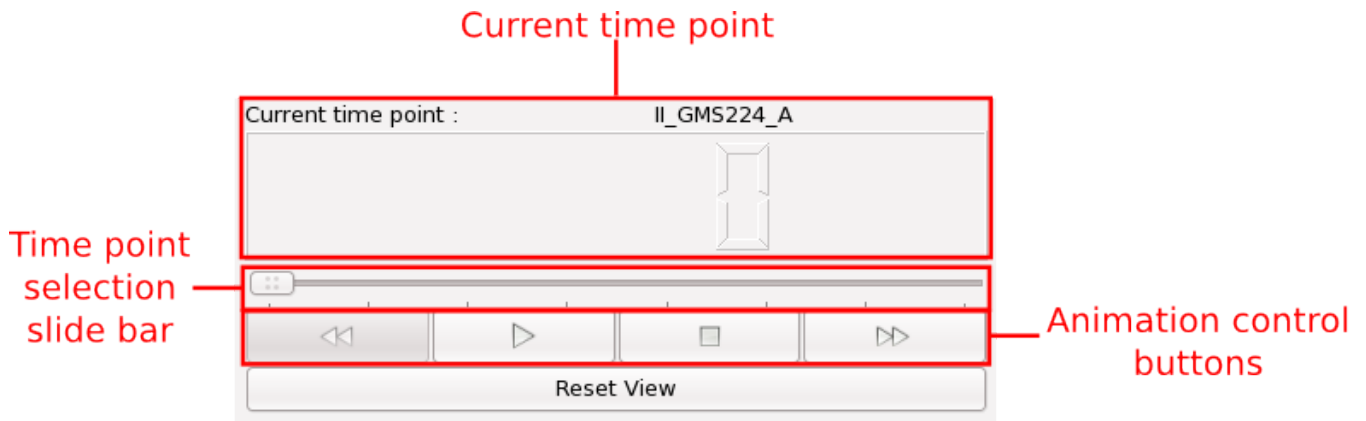







Figure 2.20: Animation control widget.

- **Current time point :** the Current time point label displays the name of the current time point and the LCD screen displays his index.
- **Time point selection slide bar :** allow user to easily jump to a given time point. Move the cursor to jump directly to the selected time point.
- **Animation control buttons :**

-  : jump to the previous time point.
-  : launch the animation from the current time point to the last. To stop animation click on the pause or on the stop button.
-  : stop the animation but keep the current time point position.
-  : stop the animation if started and go to the first time point. If animation is not running jump to the first time point.
-  : jump to the next time point.
- **Reset view :** reset the visual parameters.

### 2.2.4 Advanced options widget

This widget is only visible when advanced mode is enabled (see Advanced mode in Edit menu). It allow user to access to view, view tool and video recorder configuration widget.

### 2.2.4.1 View and view tool configuration widgets

These widgets are used to configure respectively the selected view and selected view interaction tool. When user change the selected view or the selected view tool they are automatically updated. If no configuration widget is available for a given view or view interaction tool a description widget is displayed.

Configurations widgets differs for each views and interactors so it's impossible to describe each. To know how to configure each view and interactors show their manual.

### 2.2.4.2 Video recorder configuration widget

Systrip allows to record video from a view. This widget is used to configure the record options(see Section 3.4 to know how to record video from Systrip).

Figure 2.21:

- `Output directory` : the repertory to store temporary screenshots.
- `Frames name prefix` : the prefix for temporary screenshots names.
- `Force timestamp interval` : if checked ignore the real time before two timestamps and set the value in the spin box as interval time. The value in the spin box is in millisecond.
- `Start/Stop` : begin or stop recording video from selected window.

## 2.3 Views


### 2.3.1 Metabolic view

This view is used to display networks drawings. It can display graph in two or three dimensions and enables to apply the mouse operations selected in the tool bar by directly clicking on the drawing of the graph.


#### 2.3.1.1 View operations




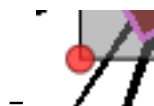
This toolbar allows to select the mouse operation you want to perform. Operations are listed and explained, from left to right of the toolbar :

-  **3D Navigation** : This tool enables the 3D navigation in a graph using the mouse movements (left button pressed); the available operations are: translate, rotate, zoom, zoom and pan. Translation is the default operation and can also be activated using the Arrow keys; rotation is activated using **Shift** key, zoom is activated using **Ctrl** key ( **Alt** key on Mac), zoom and pan is activated using the wheel of the mouse ( **APPLE** key on Mac). Warning, the last operation is 'mouse position centered'; i.e it attempts to translate the last 2D or 3D position of the mouse to the center of the view.



-  **Rectangle Selection** : Allows multiple elements selection. Elements within the selection box are selected. If **Shift** key is pressed, the newly selected elements are added to the current selection, if **Ctrl** key ( **Alt** key on Mac) is pressed, the selected elements are removed from the current selection; else they replace the current selection.

-  **Selection edition** : This tool allows to modify the current selection. Available operations are horizontal stretch, vertical stretch, all axis stretch, coordinate axis rotation and translation. If no key is pressed, coordinates are modified. If **Shift** key is pressed, only coordinates are modified. If **Ctrl** is pressed, only size is modified. A left button click outside the selection box reset the selection.




- Press on this 'circle' to rotate the selection.





- Press on this 'triangle' to change width or height of the selection.




- The 'square' is used both for resizing AND rotating the selection.

-  **Edit edge bends** : when it is selected, you can edit the bends of an edge by first selecting the edge using the mouse left button. Then a mouse left click with the **Shift** key pressed will add a new bend, moving the mouse with the left button pressed will allow to move an existing one, a mouse left click on a bend with the **Ctrl** key pressed ( **Alt** key on Mac) will remove it.

-  **Get Information** : when this operation is selected, if you click on an element of a graph (node or edge), displays all available information of that node/edge using the `Elements properties` widget tab of the `Dock widget` sub-window (see Section 2.2.2 ).

-  **Highlight neighborhood** : this interactor allows to get information regarding the neighborhood of a node by highlighting the nodes connected to it. A "Bring and Go" feature is also implemented allowing to navigate from close to close in a graph with smooth animations. First click on a node to select it, next you can either click again on it and select a neighbor to navigate to it or use the mouse wheel to modify the neighborhood selection distance.

-  **Magnifying glass** : this interactor provides a magnifying glass tool for all Tulip views. It allows to zoom on a particular area of a visualization with the help of a lens without having to modify the global zoom level. Move the mouse on the screen to move the lens. Use **Ctrl** + the mouse wheel to enlarge or reduce the lens radius. Use **shift** + the mouse wheel to improve or reduce the zoom level.

### 2.3.1.2 Contextual menu

- `Save picture as` : take a snapshot of the view and save it in the selected format.
- `Dialog` : display or hide the 3D overview.
- `Hide/Show label` : display or hide elements labels.
- `Hide/Show arrows` : display or hide edge extremities arrows. An arrow is used to show if the reaction is reversible or not. If the reaction is reversible the edge will have an arrow at each of this extremities else only one edge is visible.
- `Center view` : center the view.

### 2.3.1.3 Configuration widget

This widget is used to configure the background color for the view. To change it click on the Background color button, select the new color and click on the Apply button.

## 2.3.2 Information view

This view is used to display information from databases and to interact with. There are two states for this view : the preview mode and the detailed mode.

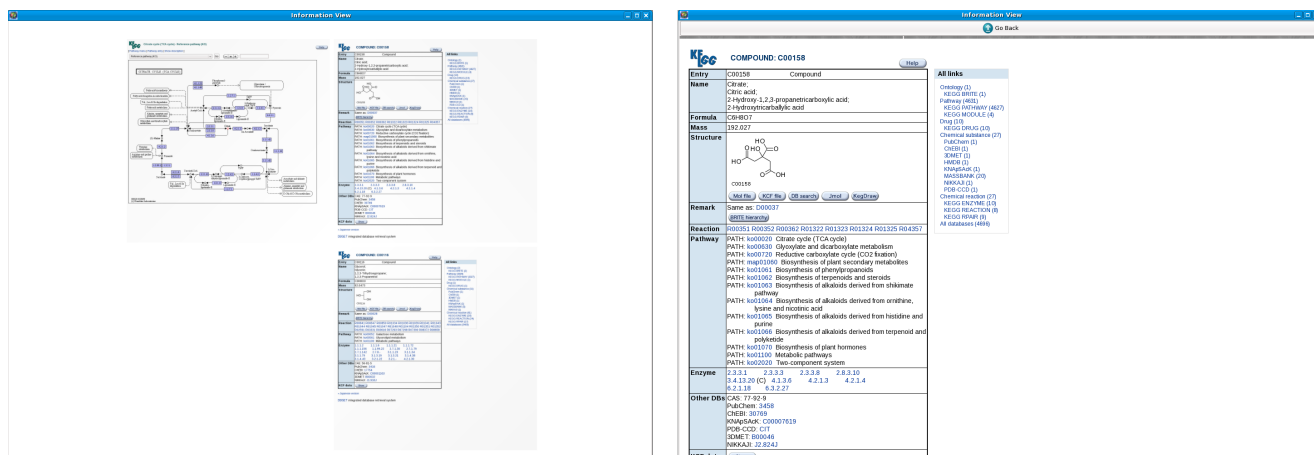


Figure 2.22: Information view two state : preview and detailed mode.

The preview mode prints a screenshot of all the selected data and when user double clicks on a screenshot the view switches to detailed. In the detailed mode the user can interact with a real HTML page. This page contains all the information found on the element in the databases. User can click on an hyperlink that will create a new screenshot on the preview mode.

### 2.3.2.1 View operations

In the preview mode user can move or zoom on preview. If user waits with the mouse pointer on a preview a tool-tip appears with the node number and the URL of this preview. To see the detailed mode for a preview user add to double click on it.

In the detailed mode the user can interact with a real HTML page. This page contains all the information found on the element in the databases. User can go back to the preview mode by clicking on the Go back button at the top of the view. User can also click on a HTML link in the page to follow them.

### 2.3.2.2 Contextual menu

There is only contextual menu on preview screen.

- Save picture as : take a snapshot of the view and save it in the selected format.

### 2.3.2.3 Configuration widget

Systrip automatically configure this view so you don't need to modify these parameters.

### 2.3.3 Molecular view

This view is used to visualize 3D molecules.

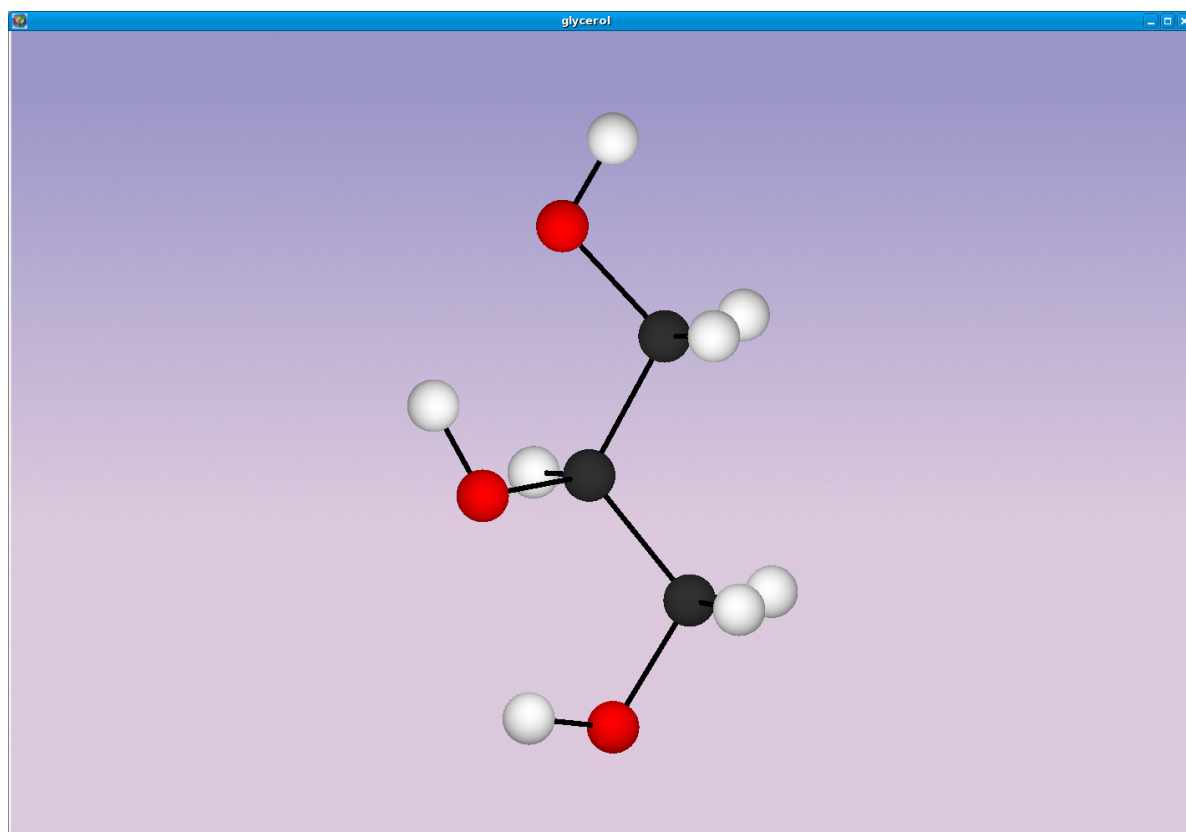


Figure 2.23: Molecular view sample.

#### 2.3.3.1 Contextual menu

- `Start/Stop auto-rotate` : start or stop the automatic rotation of the molecule.
- `Rotation Axis` : select the rotation axis for automatic rotation.
- `Center view` : center the view.
- `Save picture as` : take a snapshot of the view and save it in the selected format.
- `Dialog` : display or hide the 3D overview.

### 2.3.4 Data sets views

These views are used to represent data sets. They are specialized to visualize data evolution.

#### 2.3.4.1 Parallel coordinates view

Parallel coordinates is a common way of visualizing high-dimensional geometry and analyzing multivariate data.

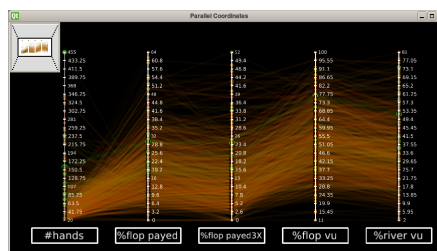


Figure 2.24: Parallel coordinates view example.

For more information see the Tulip documentation section 2.5. Tulip documentation can be found here <http://tulip.labri.fr/userHandbook/>

### 2.3.4.2 Table view

This view allow to visualize graph properties in a table form.

| Nodes | Edges       | sewBorder.Colo | sewBorder.Wid | viewColor      | viewLabel | x |
|-------|-------------|----------------|---------------|----------------|-----------|---|
| 38    | (0.0.0.255) | 0              |               | (204.204.51... | (C        |   |
| 39    | (0.0.0.255) | 0              |               | (221.221.34... | (C        |   |
| 40    | (0.0.0.255) | 0              |               | (136.136.11... | (C        |   |
| 41    | (0.0.0.255) | 0              |               | (68.68.187...  | (C        |   |
| 42    | (0.0.0.255) | 0              |               | (102.102.15... | (C        |   |
| 43    | (0.0.0.255) | 0              |               | (102.102.15... | (C        |   |
| 44    | (0.0.0.255) | 0              |               | (153.153.10... | (C        |   |
| 45    | (0.0.0.255) | 0              |               | (136.136.11... | (C        |   |
| 46    | (0.0.0.255) | 0              |               | (68.68.187...  | (C        |   |
| 47    | (0.0.0.255) | 0              |               | (170.170.85... | (C        |   |
| 48    | (0.0.0.255) | 0              |               | (68.68.187...  | (C        |   |
| 49    | (0.0.0.255) | 0              |               | (119.119.13... | (C        |   |
| 50    | (0.0.0.255) | 0              |               | (136.136.11... | (C        |   |
| 51    | (0.0.0.255) | 0              |               | (187.187.68... | (C        |   |

Figure 2.25: Table view example.

For more information see the Tulip documentation section 2.5. Tulip documentation can be found here <http://tulip.labri.fr/userHandbook/>

### 2.3.4.3 Histogram view

This view plug-in allows to create frequency histograms from graph properties (supported types are Metric and Integer).

## 2.4 Preferences dialog

This widget regroup all the configuration parameter for Systrip. Parameters are divided in three group represented by a tab in this dialog. To apply modifications done in any tab just click on the Ok button.

### 2.4.1 Visual parameters

These parameters affect all the network drawings.

- Reversible reactions node color : the color for reversible reactions.
- Reversible node color : the color for one way reactions.
- Compounds node color : the color for all the compounds.

- `Interpolate edge color from nodes` : when checked the edge color is interpolated from the color of its source node to the color of its target node.
- `Compound to reaction edges` : if the color is not interpolated, this property define the color of all edges starting from a compound and ending to a reaction.
- `Reaction to compound edges` : if the color is not interpolated, this property define the color of all edges starting from a reaction and ending to a compound.
- `Reactions label property` : the property to use as reactions label.
- `Compounds label property` : the property to use as compounds label.
- `Nodes size` : the size of node for reactions and compounds.
- `Use edge size interpolation` : if checked edge and edge extremities sizes are computed from node size and respectively `Edge size` and `Edge extremities size` parameters. If unchecked edge and edge extremities sizes are respectively `Edge size` and `Edge extremities size` parameters.
- `Edge size` : the size or size factor(if `Use edge size interpolation` parameter is checked) for edges.
- `Edge extremities size` : the size or size factor(if `Use edge size interpolation` parameter is checked) for edge extremities.

### 2.4.2 Information Table

- `Reaction properties` : the list of properties to display in the `Element properties` widget when displaying information for reactions.
- `Compound properties` : the list of properties to display in the `Element properties` widget when displaying information for compounds.
- `Query distant databases` : if checked query distant database when user display information on elements.

### 2.4.3 Metabolic plug-ins list.

This tab allow user to select available plug-ins for simple mode (see Section 2.1.1 for more information on plug-ins). Plug-ins are organized by type to see the plug-in list for a given type just select this type in the combo box at the top of the widget.

If you want to save the current list just click on the `Set as default` button. If you want to restore original selection click on the `Restore default` button.

## Chapter 3

# Features

### 3.1 Network or metabolic views visualization

User can create visualization for both of metabolic network and metabolic views.

There are two different cases : creating a new visualization and redrawing an existing visualization. To create a representation of the metabolic network just click on the draw metabolic network button. For a metabolic view just drag and drop a metabolic view item from the metabolic view widget to the workspace. To redraw an existing visualization select its windows and click on the redraw button in the Menu tool bar or on the Redraw current view action in the Metabolic network menu.

The configuration process for visualization is very simple : just choose the layout to use. To help user to choose the layout a dialog shows the list of all the layout available. If you choose a layout in the combo box the system searches if a preview for this layout is available and displays it.

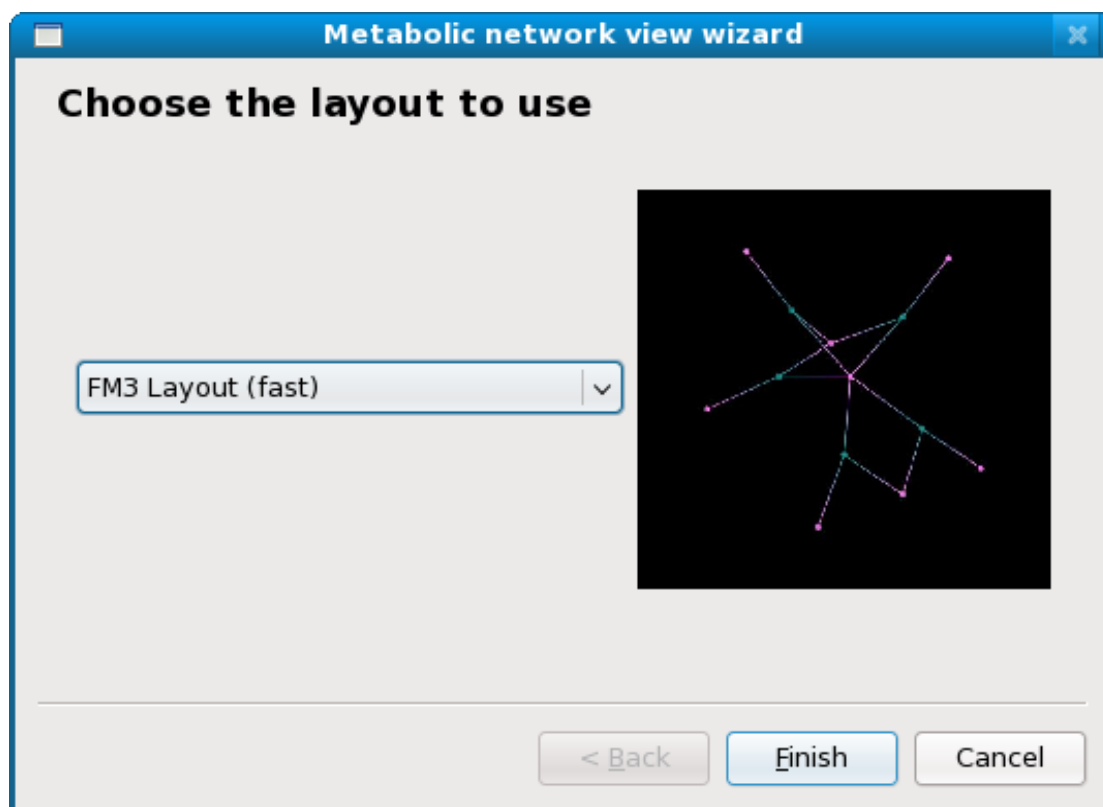


Figure 3.1: Metabolic representation configuration dialog.

Click on the `Finish` button to launch the visualization creation process.

## 3.2 Data set visualization creation

User can create various representations of data sets.

To create a new representation of a data set drag and drop a data set from the data set list to the workspace.

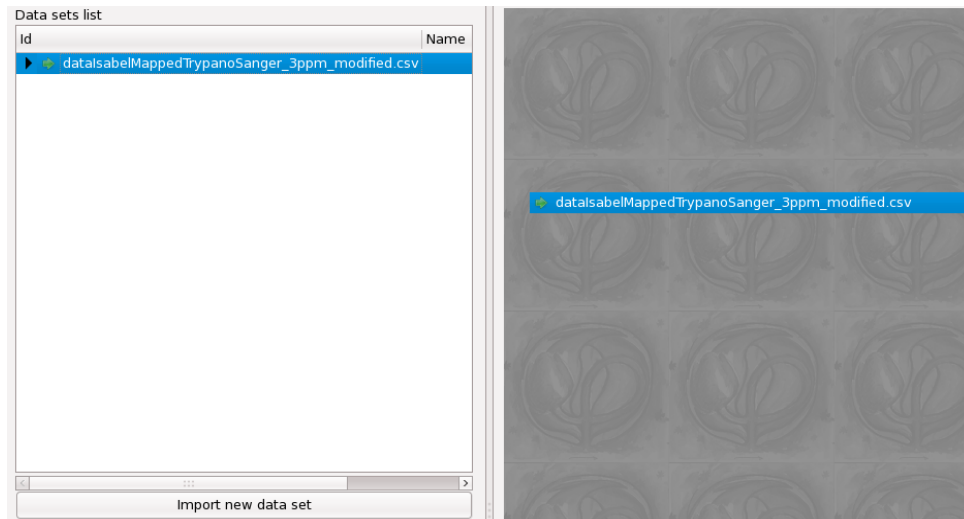


Figure 3.2: Data set representation creation.

A wizard will appear to show you the available representations. There are 3 kinds of representation :

- Parallel coordinates
- Histogram
- Table



Figure 3.3: View type selection screen.

See Section 2.3.4 for more detail on these representations.

Once the view type selected a screen with the time points to use appear. By default all the time points are selected.

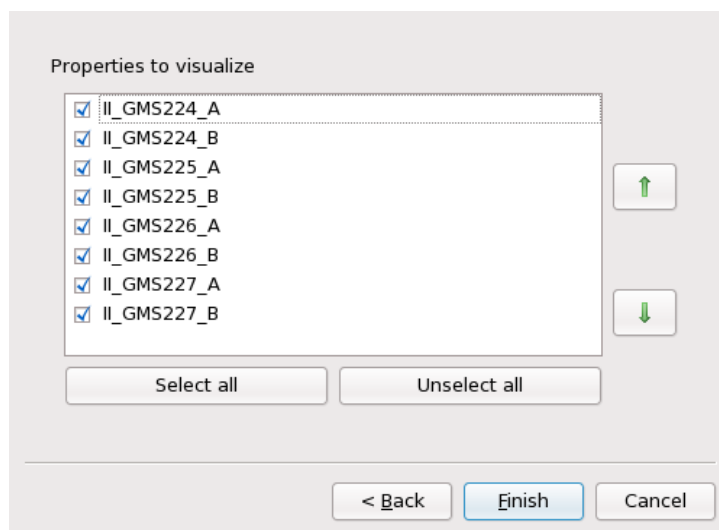


Figure 3.4: Time points selection screen.

Click on the finish button to create the representation.


### 3.3 Find tools

The tool gives a way to choose the desired property and the action you want perform regarding the current selection: Make out of the found elements a new selection, Add them to the selection, Remove them from the selection or Intersect them with the current selection.

You can search elements in the global network or just on a specific kind of element : reactions, compounds or pathway. To search in a specific type select the right menu in the Edit , Search in menu. If you use the shortcut the elements are searched in the full network.

### 3.4 Register video from view

Systrip allow user to make video from a selected window. Only one window can be recorded at the same time and it's not possible to change the recorded window during recording. Registering video slow down Systrip don't be surprised if animation or navigation are affected during recording. User can configure advanced options for recording with the Video recorder configuration widget (see Section 2.2.4.2 ). These options cannot be changed during recording.

To start recording there are two possibilities : first you can use the record shortcut in the menu  The second solution is to switch to advanced mode, to go to the video recorder configuration widget and to click on the start button (see Section 2.2.4.2 ). If there are no windows selected or if the selected windows cannot be recorded these two controls are disabled.

When beginning to record a dialog warns user about the possible loss of performance. Click on Don't show again to disable this dialog for next video recording or on Ok to just close it.

Now manipulate Systrip as you want the recording process is running. To stop recording click again on the record shortcut or on the stop button in the video recorder configuration widget. If frames were captured a file selection dialog will appear to let you choose the video file to create. Clicking on the Ok button will launch the video generation and progress bar appear to indicate the progression of the video generation. If user click on the Cancel button the video generation will be stopped.



## 3.5 Query more information in distant databases

Systrip allows user to get more detailed information from distant database. To query information on an element use the element information interactor or right click on the element in the metabolic network widget or metabolic view widget and select the `Show properties` action.

The information retrieval process is as follows : take the first database in the list and try to find the element, if no element is found go to the next database until the element is found or all the available database are queried.

User can edit the database query list to add, remove databases or change the query order. To edit this list use the `Edit database priority` action in the `Information` menu. A widget will appear to help you to edit the list.

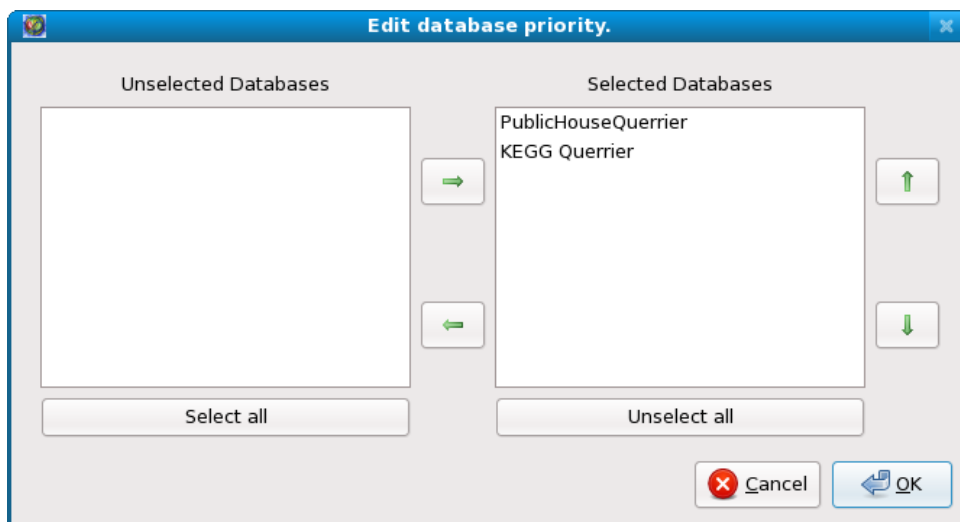






Figure 3.5: Database priority edition widget.

-  : move unselected database to selected database list.
-  : move selected database to unselected database list.
-  : increase the priority of the selected database.
-  : decrease the priority of the selected database.
- `Select all` : select all the database.
- `Unselect all` : deselect all the database.

Each database has their own parameters, user can edit them for a given database by selecting the database name in the `Database properties` menu.

### 3.5.1 KEGG

See <http://www.genome.jp/kegg/> for more information on KEGG.

There is no configuration parameters for this database.

### 3.5.2 Public house

See <http://biowarehouse.ai.sri.com/PublicHouseOverview.html> for more information on Public house.

To connect Systrip to Public House you need to use your own login and password.

To search in the database the name of your network must match with an existing organism in Public House.

The configuration parameters for this database are as following :

- host : the host of the database
- port : the port for the connection.
- database : the database name to query.
- user : the user name.
- password : the password for the user.

## 3.6 Adding new algorithms

As it's based on the Tulip framework, user can easily implements it's own algorithms to use in Systrip. To know more how to create new plug-ins see the Tulip developer manual <http://tulip.labri.fr/TulipDrupal/?q=developer-handbook> chapter 6 Plug-ins development.

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