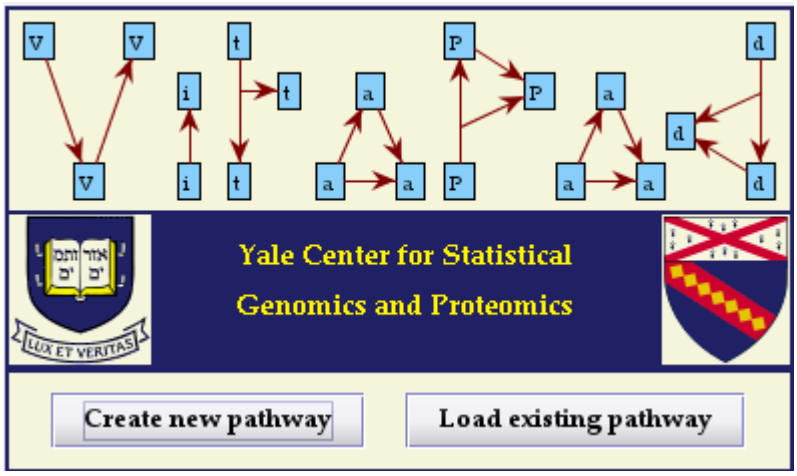
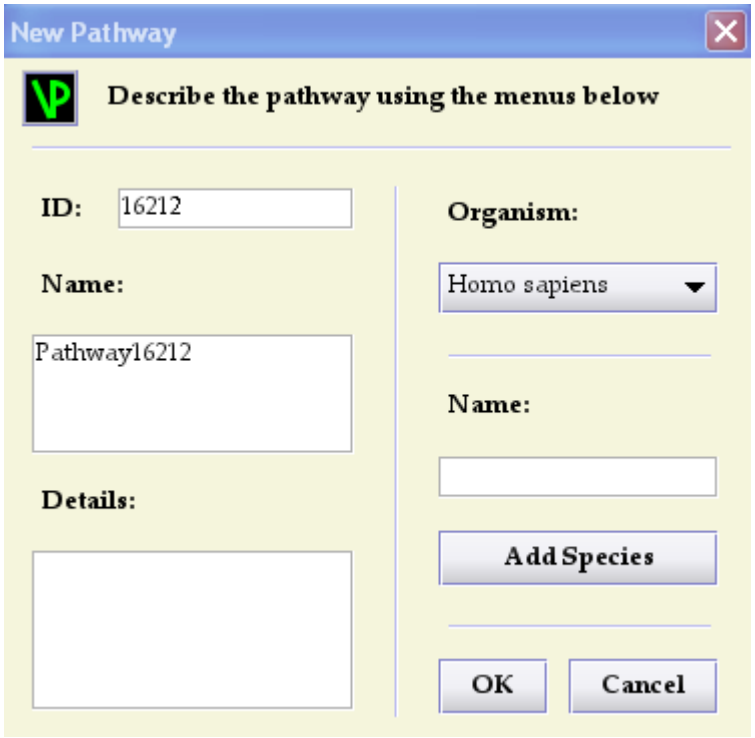
VitaPad 1.0 – Help Manual

The opening screen-

At the start of the program, you can either create a new pathway or load a previously created pathway from a file.



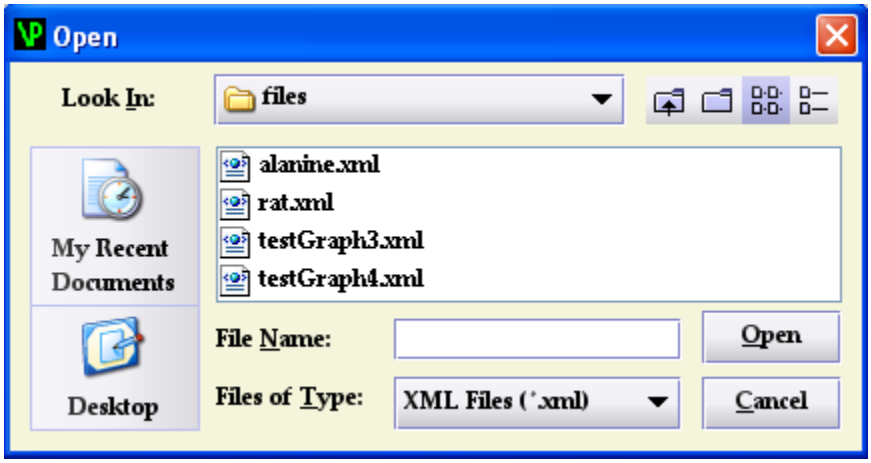
Creating a new pathway-



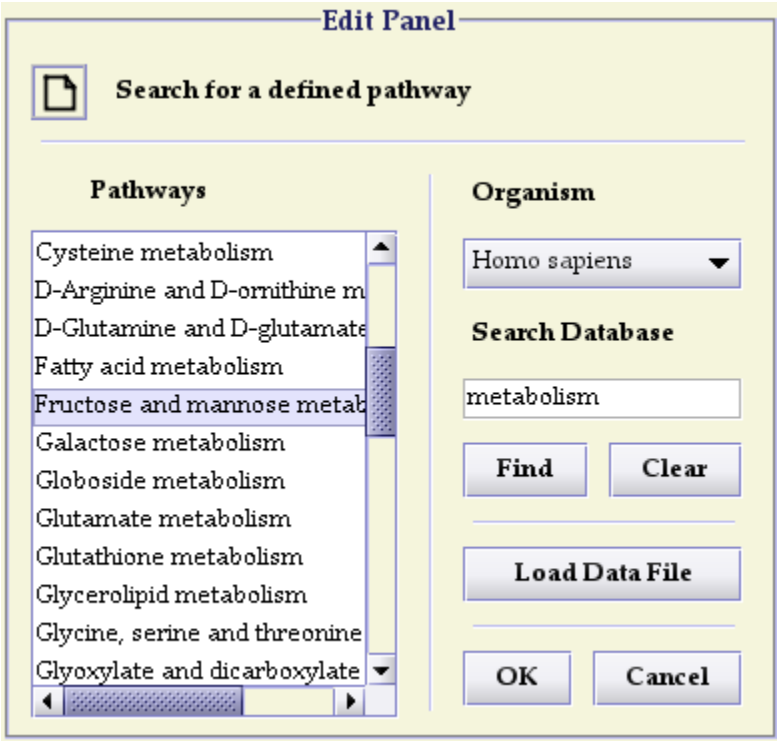
When you choose to create a new pathway, you must provide it with an ID number, a descriptive name and the organism shown. A default name is generated automatically. You can change this name at any point in creating the diagram by selecting **Edit -> Pathway Details** from the main menu.

Loading a pathway from file –

You can load a pathway from file, as long as it was generated by VitaPad in XML format. A few sample files are included in **/etc/files**.

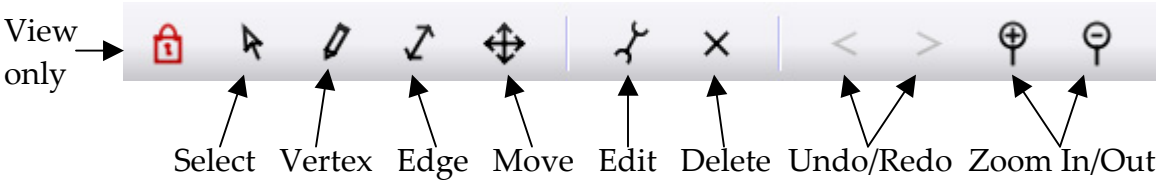


Loading a pathway from the IPA database –



You can request to have a pathway generated from the IPA (Integrated Pathway Analysis) database here at Yale. Select an organism from those currently available (*Homo sapiens*, *Mus musculus* and *Rattus norvegicus* at the moment.) Then enter a search phrase in the text field and click **Find** to search the database. Matching pathways will appear in the text box on the left. If you leave the search field blank, all available pathways for the species will be displayed. Press **Clear** to remove matches and search again. The button currently does nothing, but in the near future, you will be able to use it to import your own reaction data and generate a graph using our layout algorithm.

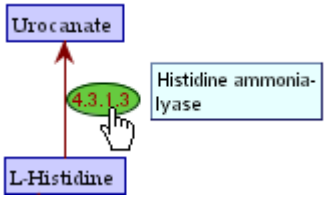
Using the toolbar –

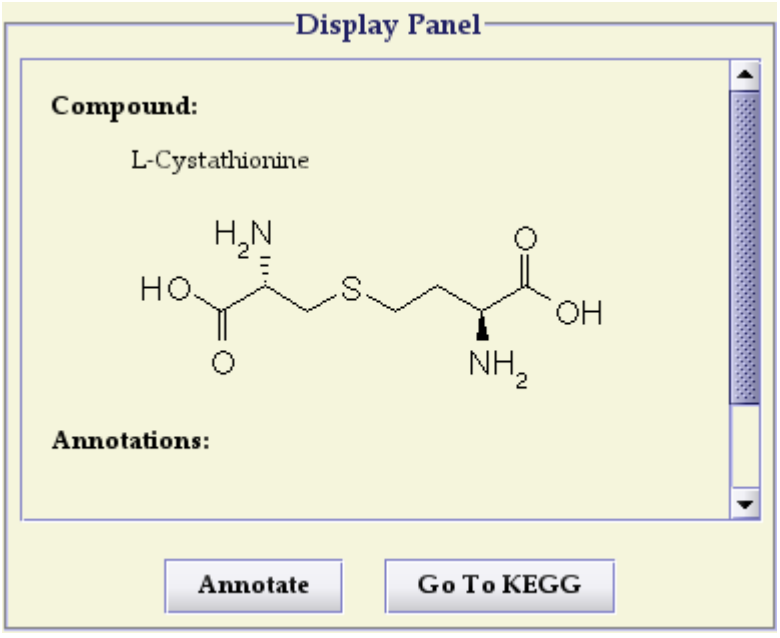


The toolbar has buttons for each of the graph views five modes of interaction (View mode, Select/Edit mode, Add Vertex mode, Add Edge mode and Move Component mode). Selecting one of these buttons toggles that mode on and the others off. The same can be done through the main menu under **Edit**. The modes will be discussed in detail below, but some mention should be made of the other buttons. The **Edit** and **Delete** buttons work as part of the Select/Edit mode only so they will be discussed there. **Undo** and **Redo** restore previous unsaved versions of the graph and can be accessed from any mode. The zoom buttons are currently inactive but will be available in future versions.

View mode –

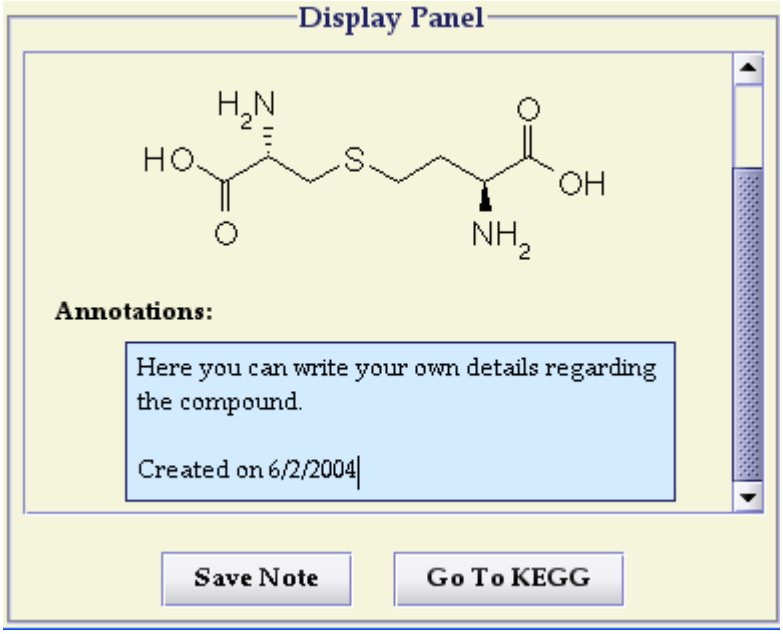
View mode is used to show specific data about the graph and elements on it. Elements cannot be added or moved in this mode. In this mode, when you mouse over an enzyme, a popup will appear showing the full name (***see right***).





Clicking on enzymes or compounds will bring up detailed information in the display panel (***see left***). If you click outside of an enzyme or compound, information for the pathway itself will be displayed. If you click on Go To KEGG, a browser window will pop up showing the KEGG web page with further details

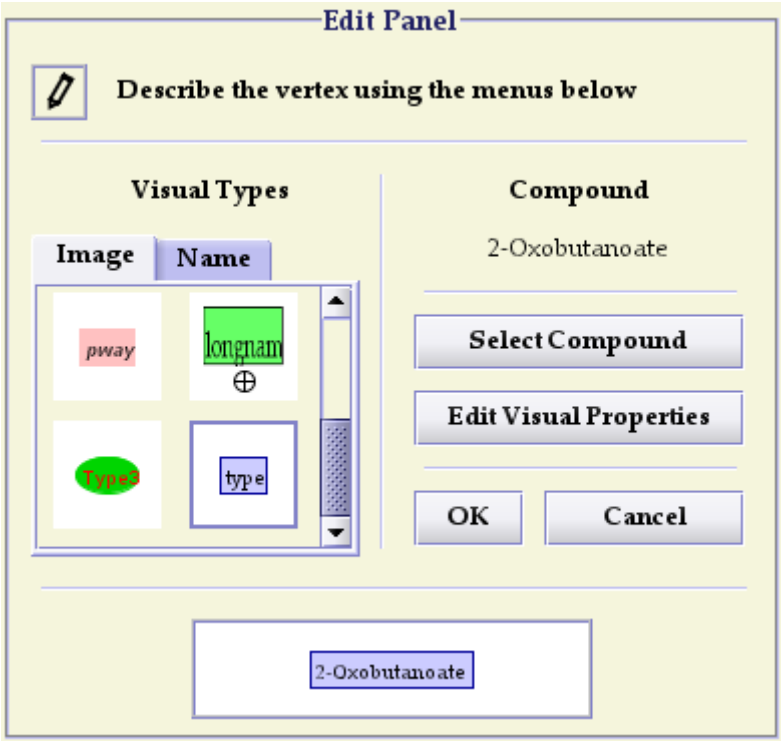
about the compound, enzyme or pathway displayed. If you click on **Annotate**, you can provide additional information to be saved with your pathway (***see right***).



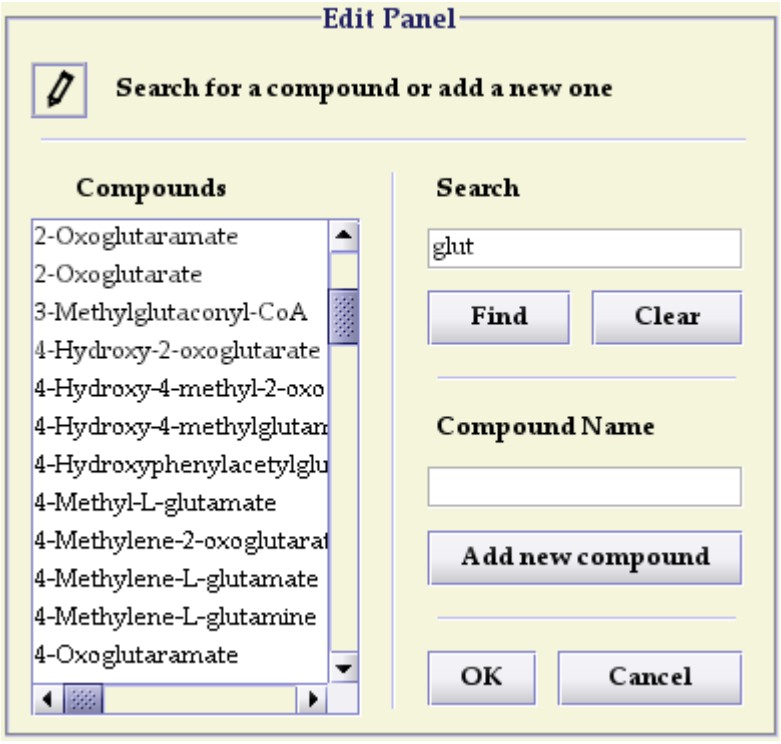
Select/Edit mode –

This mode is used to modify or delete existing pathway components. Click on the edges or vertices you wish to modify, holding down the shift key to select more than one if you wish, and press the X icon to delete or the wrench icon to edit. You can also select all compounds or links using the main menu (**Edit -> Select All -> Compounds** or **Links**. Editing uses the same dialogs as for adding vertices or edges, so I will discuss them below. Please note also that enzymes, genes and expression values get edited along with the edge they are connected to, not separately.

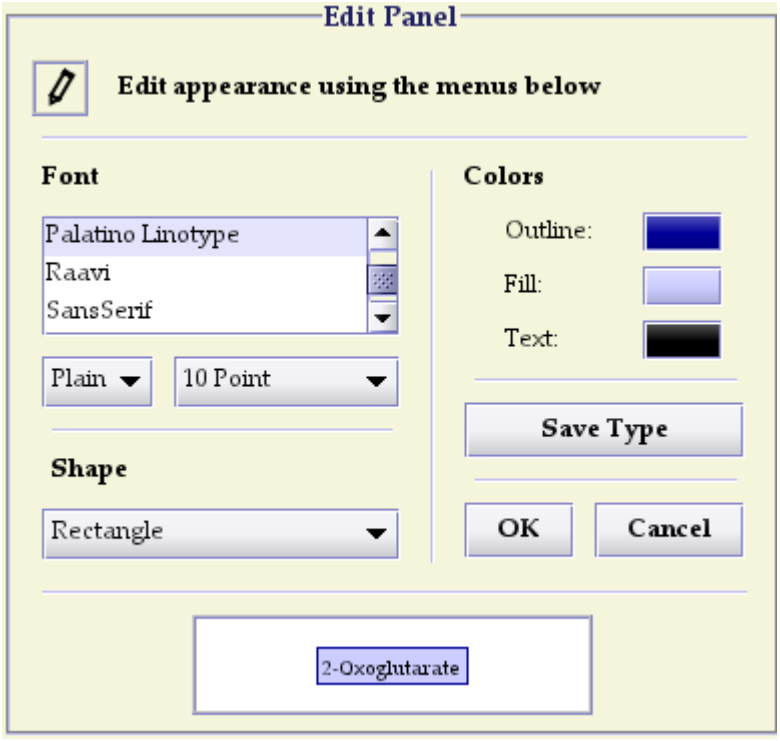
Add Vertex mode –



In this mode, if you click on the graph, an animated plus cursor will appear at the spot the vertex will be located and the dialog on the right will appear in the edit panel.
The box on the left shows a thumbnail view of saved visual types that can be selected for the object. The window at the bottom of the dialog shows a preview of how the selected compound will appear using this type. For types too large to appear in a thumbnail (e.g. those using a large font), you can see a full-sized view by mousing over the scope icon.
New visual types can be created by clicking on **Edit Visual Properties**. To select a different compound, click on **Select Compound**.



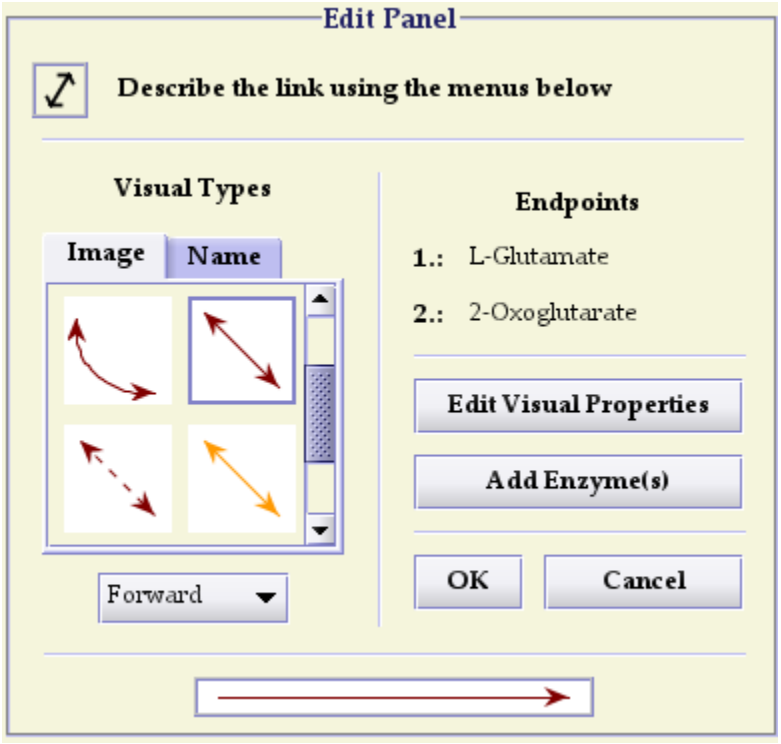
The dialog to select a compound is pictured on the left. Type a search phrase in the text field and matching compounds from the IPA database will be returned. If you leave the field blank, all compounds will be returned. If you cannot find your compound, you can type a name in the lower text field and click **Add new compound**. The compound will now be stored along with your graph.



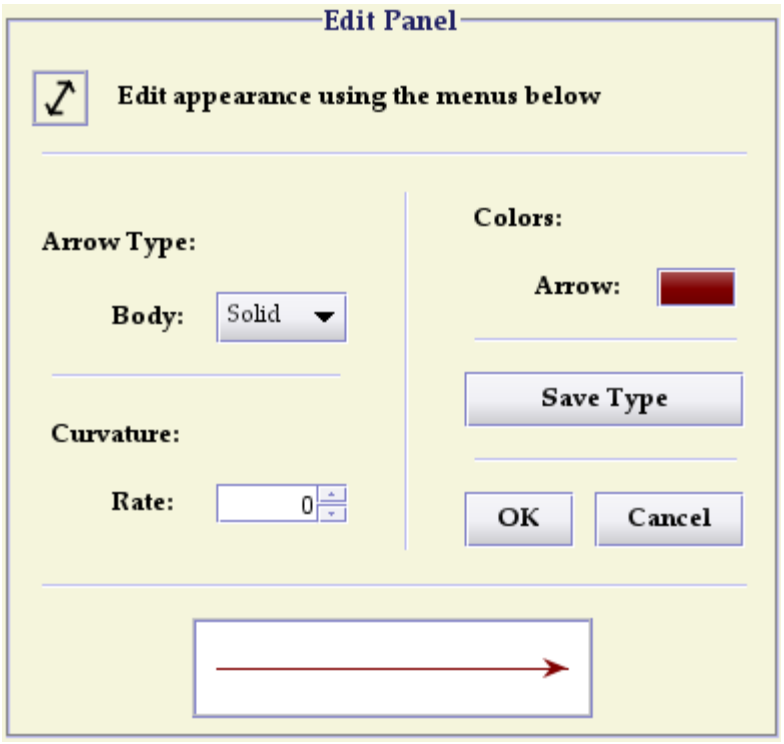
The dialog to edit vertices is pictured at left. The font box allows you to select from any font available on your system. With the combo box below, you can select style (plain, bold or italic) and point size. Below **Shape**, you can select from the following: rectangle, ellipse and rounded rectangle. In future versions, more shapes will be made available as well as the ability to create a custom shape. You can choose the color scheme for the compound, by clicking on the appropriate colored button. Once the appearance is to your liking, you can save it to disk by clicking on **Save Type**. Now, the shape will be available for ready access from the thumbnail menu in the Add Vertex dialog. The window at the bottom of the dialog shows a preview of your customized type.

Add Edge mode –

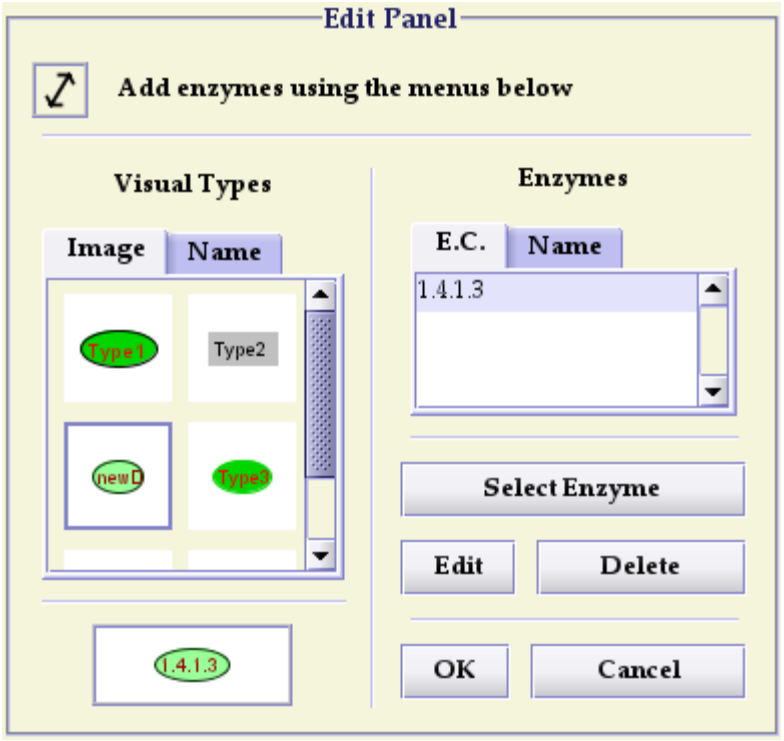
To add an edge, click the first element on the graph you wish to connect and then the second. Usually, you will connect two vertices, but it is also possible to draw an edge to another edge. In this case you would click an existing edge on the graph. The dialog for adding edges is similar to that for adding vertices. Again there is a thumbnail menu containing default and



previously saved types and a preview window. Below the thumbnail menu, is a combo box allowing you to specify the direction of the arrow. The options are forward: endpoint 1 to endpoint 2, backward: endpoint 2 to endpoint 1, both ways and neither for an undirected edge. If one or both of your endpoints is another edge, you can select the relative placement of the new edge (0.5, or at the midpoint, is the default). You can add enzymes to the edge by clicking on **Add Enzyme(s)** and change the appearance by clicking **Edit Visual Properties**.

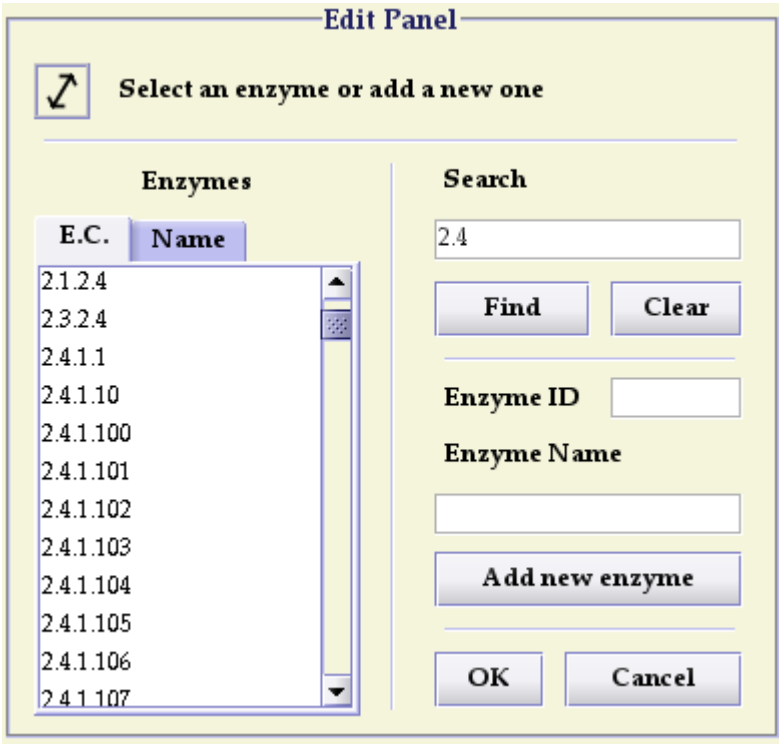


The dialog to edit edges is picture on the left. The arrow type combo box allows you to select either a solid or dotted line. In the future, additional types, such as the flat-ended edge for inhibition reactions, will be available as well as the ability to draw your own edge type. The rate of curvature takes values from 0 to 1. At this point, anything higher than 0 will apply the same degree of curvature (i.e., a line is either curved or it is not). This feature is currently rather limited, but it will be enhanced in future versions. Please note also that you cannot currently attach an enzyme to a curved edge. You can choose the color of the edge by selecting the colored button. By clicking **Save Type**, you can save your custom type to disk. Now this type will be easily available from the thumbnail menu in the Add Edge dialog.



The dialog to add enzymes is pictured on the left. This menu is quite similar to that for adding vertices, so I will summarize briefly. The thumbnail menu shows saved types. The **Edit** button allows you to customize the enzyme's appearance using the same menu as that to edit the appearance of vertices. Clicking **Select Enzyme** brings up a dialog to choose an enzyme. **Delete** will remove the highlighted enzyme from the edge. Note that an edge can contain any number of enzymes, including none.

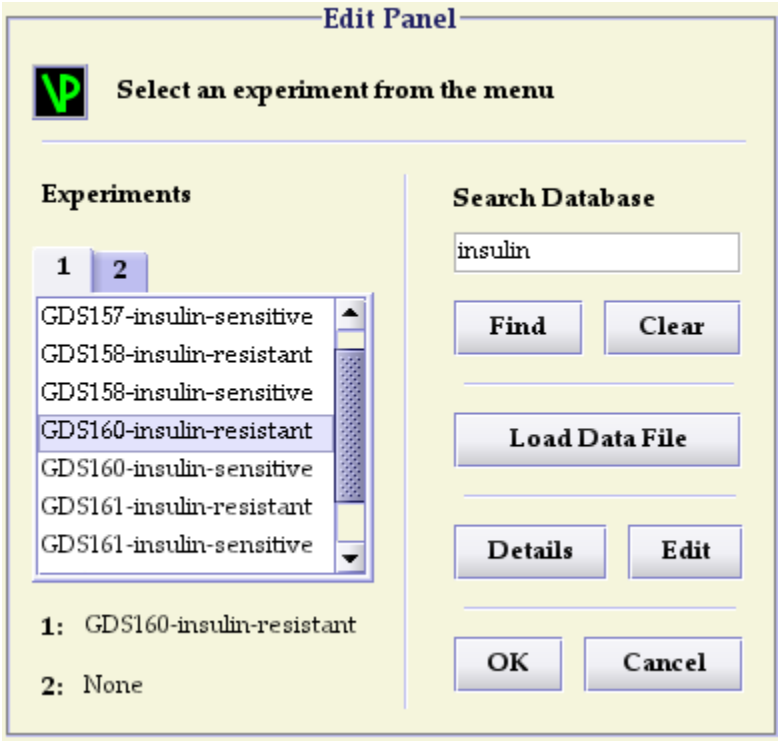
The dialog to select an enzyme is show on the right. To select an enzyme, enter search criteria in the text field below **Search** and matching enzymes from the IPA database will be shown. You can search either a numerical sequence in the E.C. number or a string from the full name of the enzyme. If your enzyme is not found, you can enter a new one by filling in the **Enzyme ID** and **Enzyme Name** fields and clicking **Add new enzyme**. Your new enzymes will now be stored along with your graph.



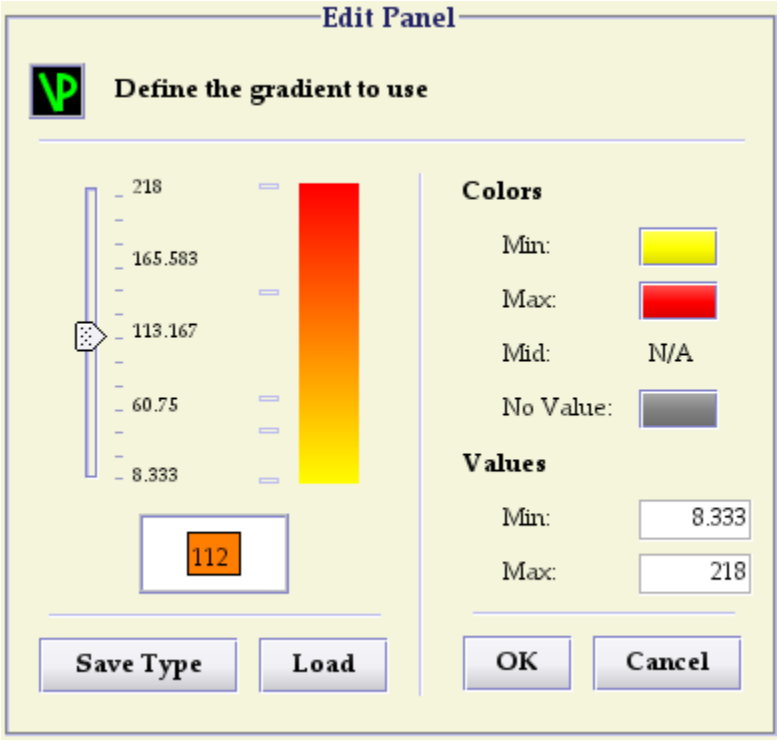
Move mode –

In move mode, you can move elements on the graph by simply clicking on vertices and dragging them to the new location. The graph is updated as the element is moved. As the vertex moves, the edges connected to it move in conjunction. Please note that decorations such as enzymes, genes and expression values move with the edge they are attached to and cannot be moved separately.

Loading experiment data –



To map experimental data onto a pathway diagram, select File -> Load Experiment from the main menu. The dialog for selecting an experiment is shown on the right. You can select load either one or two experiments to display. If you select two, the value displayed will be the ratio of values for the two (Experiment 1 / Experiment 2). To load an experiment from the IPA database, enter search criteria from the text field under **Search Database** and click **Find**. All matching experiments are displayed in the text box on the left. If you leave the field blank, all available experiments will be displayed. In the near future, you will be able to enter your own experiment data by clicking on **Load Data File**. Clicking on **Details** will open a text box with a description of the experiment.



Before you can display the experiment data, you must click on Edit to create the gradient pattern to color the values. The Edit Gradient dialog is shown on the left. The current gradient is shown on the left side of the dialog along with a slider showing the range of values. A small rectangle is shown for each data value in the experiment and a preview window indicates how the data value will appear using the gradient. By moving the slider, you can get an idea of how your data values will appear. You can adjust the color values used to define the gradient by clicking on the colored buttons. Mid is the color used to represent a 1 : 1 ratio for two experiments. In addition, you can adjust the minimum and maximum values for the gradient using the corresponding text fields. By default, these are set to the maximum and minimum values of the experiment data. If you click on **Save Type**, you can save your custom to disk for future use.

Saving your pathway –

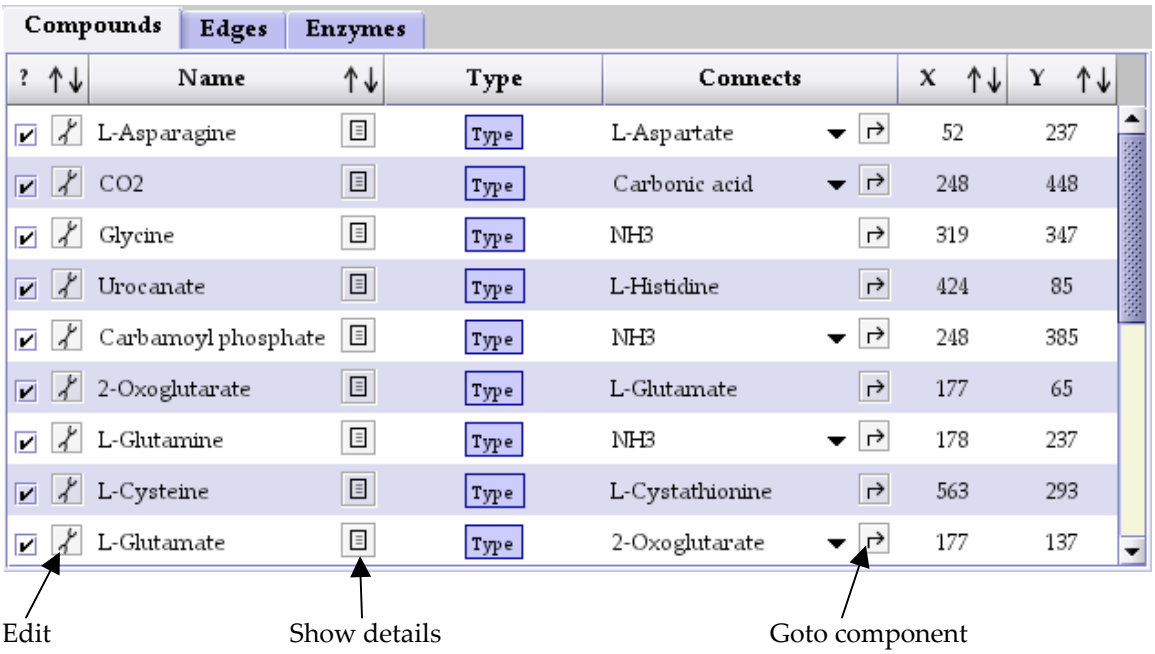
You can save your pathway in two ways: as an image or as data. To save as data select **File -> Save File** from the main menu. This will save the file in our custom XML format and will allow you to load and modify the data at a later time. To save a PNG image of the graph, select **File -> Save Image** from the main menu.

Printing your pathway –

You can send an image of your graph by selecting **File -> Print** from the main menu. The print preview option (**File -> Print Preview**) is currently not functional, but will be enabled for future releases.

Table View -

The table view for the graph can be accessed by selecting Edit -> Table View from the main menu. Please note that the table view is primarily for display purposes at this point. In the near future, you will be able to edit graph components using the same dialogs as for the graph view and select elements to include by clicking on their check box. Currently, you can sort the elements in ascending or descending alphabetical order using the arrow icons in the column header cells.



The figure above shows the table view for compounds; views for edges or enzymes can be seen by clicking on the appropriate tabs.

Additional information –

Please contact me if you have any questions or comments regarding this software:

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