



MetScape Plugin User Guide

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OVERVIEW

About data sources

MetScape is a plug-in for Cytoscape, the bioinformatics network visualization tool. The plug-in can be used to visualize and interpret metabolomic data in the context of human metabolic networks.

MetScape provides a metabolite database developed by extracting and integrating information from the following sources:

- NCIBI HUMDB Database—<http://portal.ncibi.org/gateway/tryourtools.html>
- Edinburgh Human Metabolic Network (EHMN)—<http://www.ehmn.bioinformatics.ed.ac.uk/>
- KEGG COMPOUND Database—<http://www.genome.jp/kegg/compound/>

Workflow overview

With MetScape, you can:

- Trace the connections between metabolites and genes.
- Visualize compound networks and display compound structures, as well as information for reactions, enzymes, genes, and pathways.
- Upload experimental data to visualize and explore compound networks over time or in varying experimental conditions.

The basic steps in the workflow include:

1. [Enter data](#). You can type or paste a list of compounds, upload a file of containing experimental data, or start from a biological pathway.
2. [Select compound and reaction attributes](#). Choose which attributes to display in a table as you work with a visual network graph.
3. Explore the visual network and table of attributes:
 - [Expand](#) and [collapse](#) a network.
 - [Create a subnetwork](#).
 - Sort and filter data, including the [filtering of reactions by pathway](#).
 - Visualize your data in a wide variety of network layouts provided by Cytoscape.
 - Use color, size, and other effects to visually reflect a set of attribute values.

4. [Display additional information](#) not included as compound or reaction attributes.
5. [Save your session and reopen it later.](#)

INSTALLING CYTOSCAPE AND THE METSCAPE PLUGIN

You can use the MetScape plugin for Cytoscape in one of two ways:

- **By launching Cytoscape and the MetScape plugin from MiMI Web.** With this method, you launch a temporary copy of Cytoscape and the MetScape plugin from a Compound Details page after performing a search on MiMI Web. Use this method when you don't have the administrative privileges to install software on your computer. You will not have access to other plugins when you use this method.
- **By installing Cytoscape and the MetScape plugin on your local computer.** With this method, you can use other plugins that work with MetScape data, such as Shortest Path and MCODE.

Launching Cytoscape and the MetScape plugin from the Web

To launch Cytoscape and the MetScape plugin from MiMI Web:

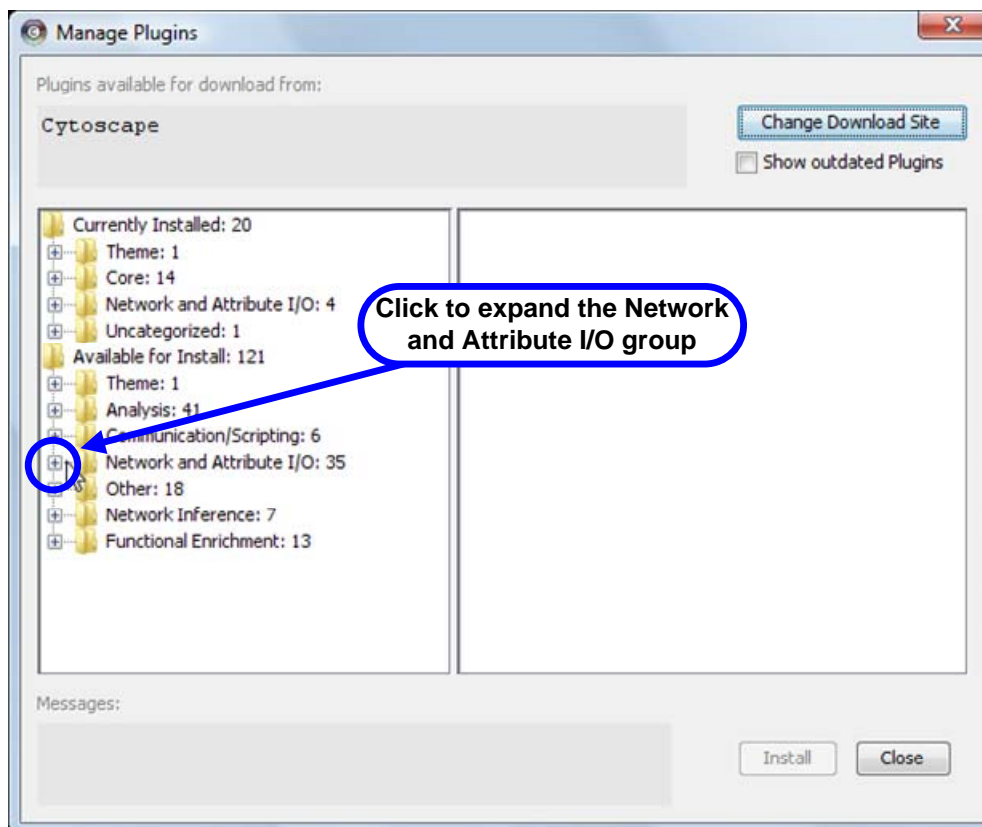
1. Go to <http://mimi.ncibi.org/MimiWeb/upload-page.jsp>.
2. Click the **Browse** button and select a text file containing compound IDs, one per line.
3. Click the **Copy to Text Box** button.
4. For **Select type**, choose **Cids**.
5. Click the **MiMI Search** button.
6. Click a compound ID link.
7. On the **Compound Details** page, click the **View in Metscape** link.

After launching the Web version, you can do anything described in this User Guide.

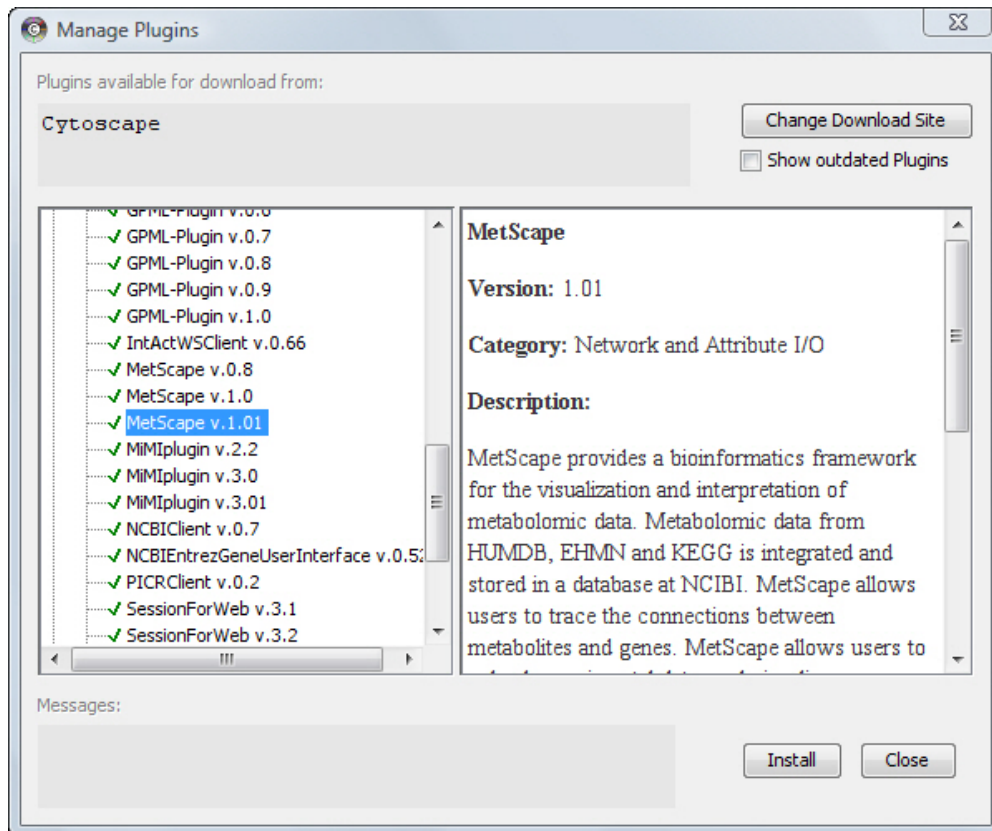
You can save your Cytoscape session on your local computer and reopen it at a later time after launching the application from MiMI Web again.

Installing Cytoscape and the MetScape plugin on your local computer

1. Install Cytoscape on your computer. For more information, go to:
 - The Cytoscape website at <http://cytoscape.org/>.
 - or*
 - The NCIBI Virtual Workshop page at <http://portal.ncibi.org/gateway/virtual-workshop.html>.
2. After Cytoscape is installed, start the application.
3. To install the MetScape plugin, select **Plugins → Manage Plugins** from the Cytoscape menu.
4. Under **Available for Install**, click the + box to expand the **Network and Attribute I/O** group.



5. Find and click the most recent version of the MetScape plugin.



6. Click **Install**.
7. When installation is complete, click **Close**.

A **MetScape** option is added to the Cytoscape **Plugins** menu.

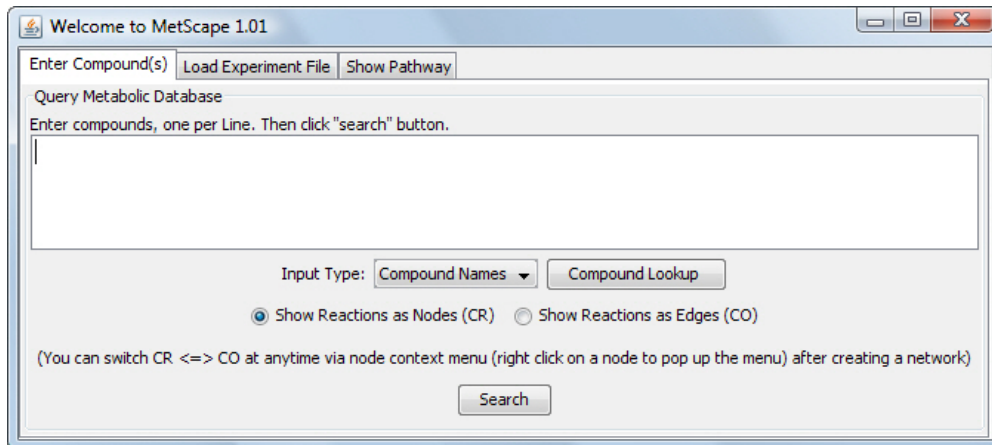
ENTERING DATA

1. To begin a Cytoscape session with the MetScape plugin, first start Cytoscape.
2. Select **Plugins** → **MetScape** → **Build Network** from the Cytoscape menu.
3. Choose one of the following methods to get started.

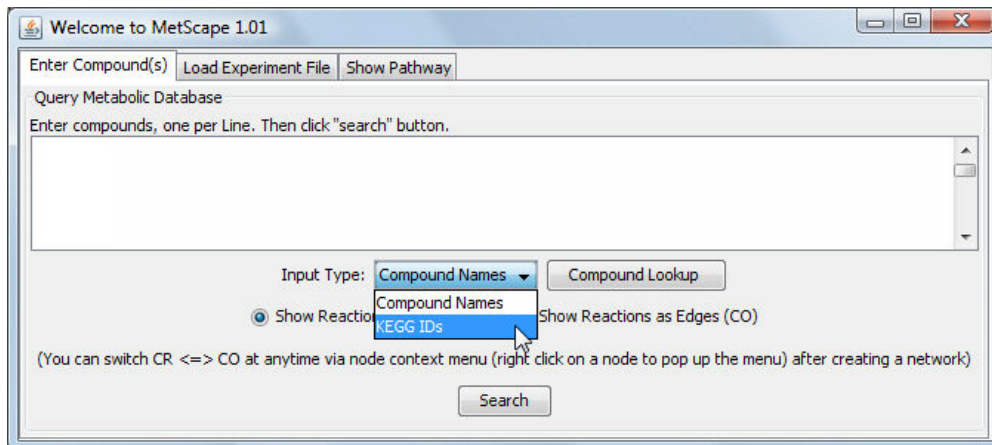
Option 1: Enter a list of compounds

Use to explore a network of compounds and reactions, starting from a list of compounds.

1. Click the **Enter Compound(s)** tab.



2. To identify compounds, you can enter compound names or KEGG compound IDs. To enter KEGG IDs, select **KEGG IDs** from the **Input Type** dropdown:



- In the text box, enter or paste compound names or KEGG IDs, each on its own line.

Examples:

<i>Compound names</i>	<i>KEGG compound IDs</i>
glutathione	C00051
glucose	C00293
fructose	C01496
creatinine	C00791
d-mannose	C00159
adenosine	C00212
taurine	C00245
myo-inositol	C00137
inosine	C00294
beta-alanine	C00099
urate	C00366
nicotinamide	C00153
uridine	C00299
n-acetyl-beta-d-glucosaminylami	C01239
n-acetyl-d-glucosamine	C00140

If you need to look up a compound name or ID, click **Compound Lookup**. On the resulting NCIBI compound lookup page, use your browser's **Find (Ctrl-F)** command to enter the name or ID to find the row that contains both.

Compound		
Compound ID	Name Type	Compound Name
CE5935	synonym	((2S),(6R),10)-trimethylundecanoyl-CoA
CE5935	synonym	((2S),(6R),10)-trimethylundecanoyl-CoA sym (2S,6R,10)-trimethylundecanoyl-CoA
CE3134	synonym	(-)-5-(3',4',5'-trihydroxyphenyl)-gama-valerolactone
CE3134		(-)-5-(3,4,5-trihydroxyphenyl)-gama-valerolactone
CE3134	primary_name	(-)-5-(3,4,5-trihydroxyphenyl)-gama-valerolactone
CE3126	synonym	(-)-5-(3,4,5-trihydroxyphenyl)-gama-valerolactone sulfate
CE3134	synonym	(-)-delta-(3',4',5'-trihydroxyphenyl)-gama-valerolactone
CE3134	synonym	(-)-delta-(3,4,5-trihydroxyphenyl)-gama-valerolactone
CE3811		(-)-delta-(3',4',5'-trihydroxyphenyl)-gama-valerolactone 3',4',5'-trisulfate
CE3811	primary_name	(-)-delta-(3',4',5'-trihydroxyphenyl)-gama-valerolactone 3',4',5'-trisulfate
CE3809		(-)-delta-(3',4',5'-trihydroxyphenyl)-gama-valerolactone 3',4'-disulfate
CE3809	primary_name	(-)-delta-(3',4',5'-trihydroxyphenyl)-gama-valerolactone 3',4'-disulfate
CE3810		(-)-delta-(3',4',5'-trihydroxyphenyl)-gama-valerolactone 3',5'-disulfate
CE3810	primary_name	(-)-delta-(3',4',5'-trihydroxyphenyl)-gama-valerolactone 3',5'-disulfate
CE3126		(-)-delta-(3',4',5'-trihydroxyphenyl)-gama-valerolactone 3'-sulfate
CE3126	primary_name	(-)-delta-(3',4',5'-trihydroxyphenyl)-gama-valerolactone 3'-sulfate

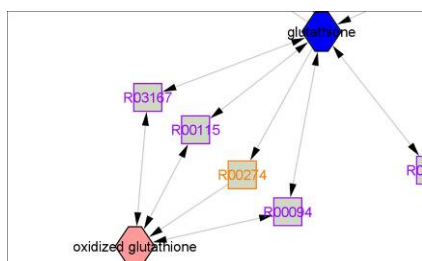
- Select a network style by selecting either **Show Reactions as Nodes** or **Show Reactions as Edges**.

With **Show Reactions as Nodes**, the network will consist of the queried compounds, reactions in which they participate, and any other compounds involved in those reactions, all shown as nodes.

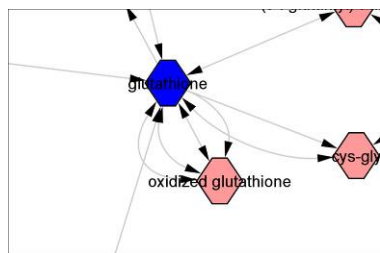
With **Show Reactions as Edges**, the network will consist of the queried compounds and the nearest-neighbor compounds shown as nodes, and the reactions they share shown as edges.

Examples of resulting networks:

Reactions and compounds as nodes:



Reactions as edges, compounds as nodes:



5. Click **Search** to query the metabolic database and create the network.

Option 2: Load an experiment file

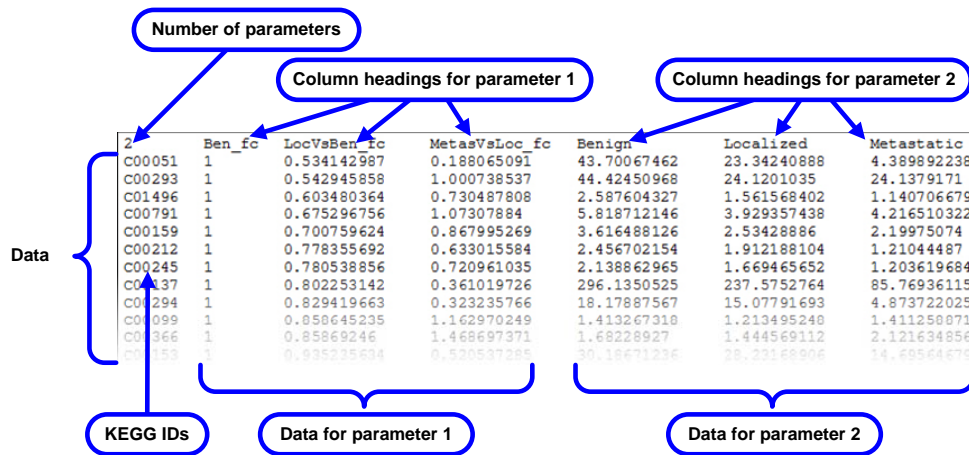
Use to upload experimental data to visualize and explore compound networks over time or in varying experimental conditions.

The data file must meet the following requirements:

- The data should be normalized.
- The file must be a text file with:
 - Columns separated by tabs.
 - Rows separated by new lines (each row on its own line).
- The first row must be a heading row, in which:
 - The first column indicates the number of parameters.
 - The remaining columns in the first row are column headings to label the data, one set of column headings for each parameter.

- All other rows contain experimental data, in which:
 - The first column contains a KEGG compound ID.
 - The remaining columns contain data, one set of data values for each parameter.

Example:

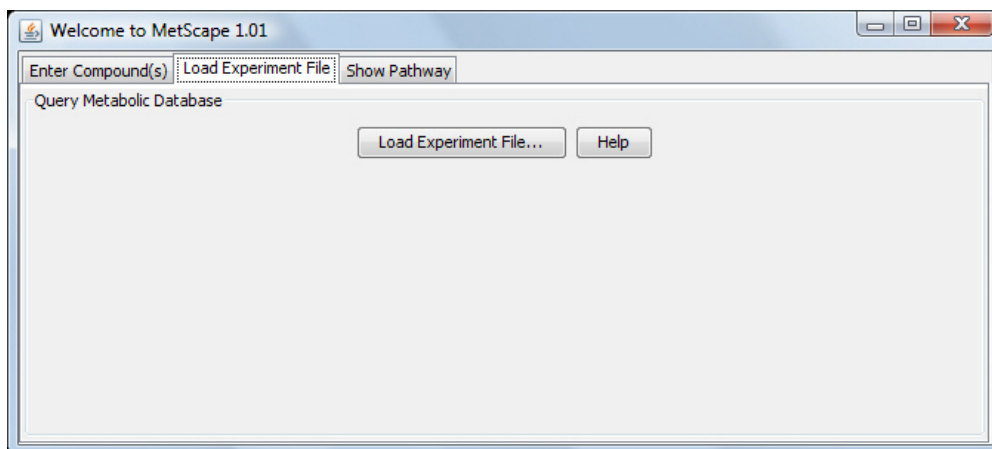


	2	Ben_fc	LocVsBen_fc	MetasVsLoc_fc	Benign	Localized	Metastatic
C00051	1	0.534142987	0.188065091	43.70067462	23.34240888	4.389892238	
C00293	1	0.542945858	1.000738537	44.42450968	24.1201035	24.1379171	
C01496	1	0.603480364	0.730487808	2.587604327	1.561568402	1.140706679	
C00791	1	0.675296756	1.07307884	5.818712146	3.929357438	4.216510322	
C00159	1	0.700759624	0.867995269	3.616488126	2.53428886	2.19975074	
C00212	1	0.778355692	0.633015584	2.456702154	1.912188104	1.21044487	
C00245	1	0.780538856	0.720961035	2.138862965	1.669465652	1.203619684	
C00437	1	0.802253142	0.361019726	296.1350525	237.5752764	85.76936115	
C01294	1	0.829419663	0.323235766	18.17887567	15.07791693	4.873722025	
C00099	1	0.858645235	1.162970249	1.413267318	1.213495248	1.411258871	
C00366	1	0.85869246	1.468697371	1.68228927	1.444569112	2.121634856	
C00553	1	0.895235634	0.520537285	39.18671236	28.23168906	14.69564678	

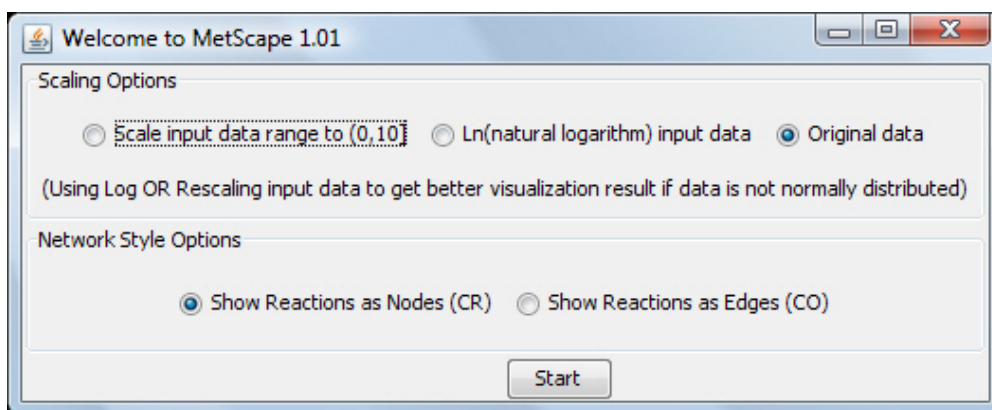
In this example, the column headings are:

- **Ben_fc:** Benign fold change
- **LocVsBen_fc:** Localized vs. benign fold change
- **MetasVsLoc_fc:** Metastatic vs. localized fold change
- **Benign:** Concentration
- **Localized:** Concentration
- **Metastatic:** Concentration

1. Click the Load Experiment File tab.



2. Click the **Load Experiment File...** button.
3. Navigate to the text file containing experiment data and click **Open**. The **Scaling Options** dialog appears:



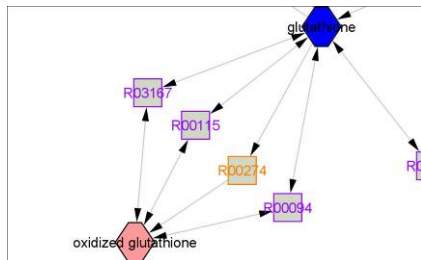
4. Optionally, select a scaling option, which may improve the visual representation of changes in data:
 - **Scale input data range to (0,10)**. Use this scaling method when the range of the input data is large or not normally distributed.
 - **Ln(natural logarithm) input data**. Use this method when the range of the input data is large.
 - **Original data**. Use this method to use original data with no scaling.
5. Select a network style by selecting either **Show Reactions as Nodes (CR)** or **Show Reactions as Edges (CO)**.

With **Show Reactions as Nodes (CR)**, the network will consist of the queried compounds, reactions in which they participate, and any other compounds involved in those reactions, all shown as nodes.

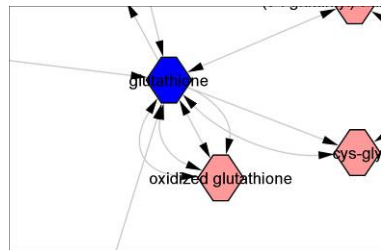
With **Show Reactions as Edges (CO)**, the network will consist of the queried compounds and the nearest-neighbor compounds shown as nodes, and the reactions they share shown as edges.

Examples of resulting networks:

Reactions and compounds as nodes:



Reactions as edges, compounds as nodes:



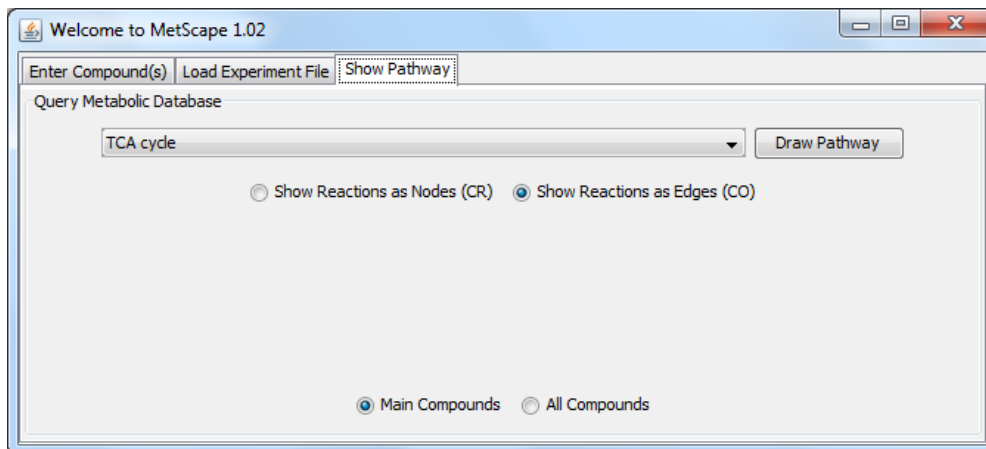
6. Click **Start** to query the metabolomics database and create the network.

To work with your experiment data, see "[Visualizing Changes in Experimental Data.](#)"

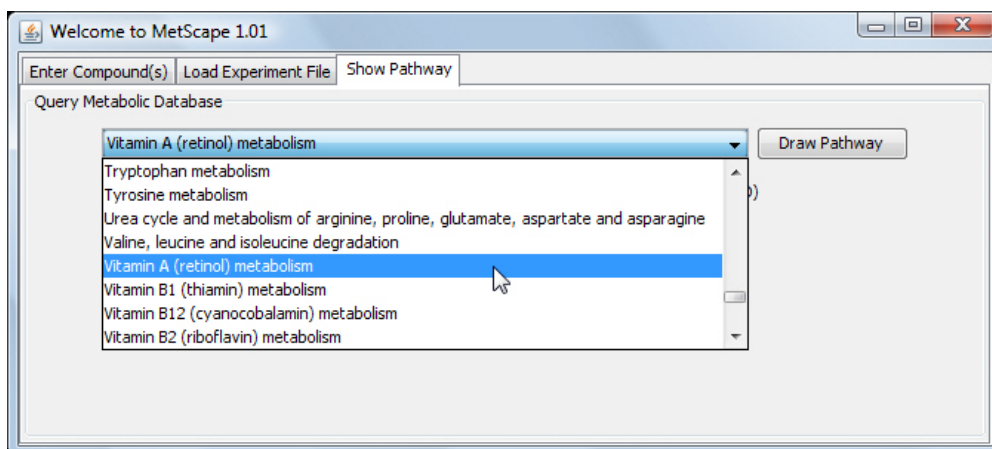
Option 3: Select a pathway

Use to view all the compounds and reactions associated with a metabolic pathway.

1. Click the **Show Pathway** tab.



- Select a specific pathway from the drop-down list, or select **All** at the top of the list.



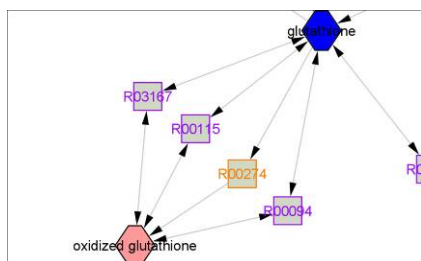
- Select a network style by selecting either **Show Reactions as Nodes** or **Show Reactions as Edges**.

With **Show Reactions as Nodes**, the network will consist of the queried compounds, reactions in which they participate, and any other compounds involved in those reactions, all shown as nodes.

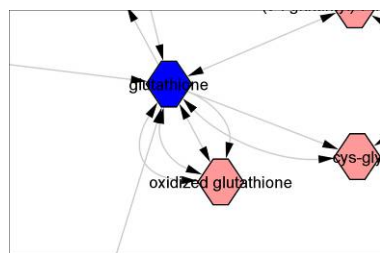
With **Show Reactions as Edges**, the network will consist of the queried compounds and the nearest-neighbor compounds shown as nodes, and the reactions they share shown as edges.

Examples of resulting networks:

Reactions and compounds as nodes:



Reactions as edges, compounds as nodes:



- Click **Draw Pathway** to create the network.

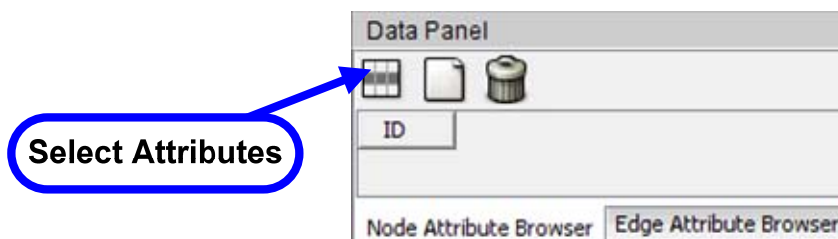
CHOOSING ATTRIBUTES FOR DISPLAY IN THE DATA PANEL

Attributes of compounds and reactions you have selected in the network appear in the Cytoscape Data Panel.

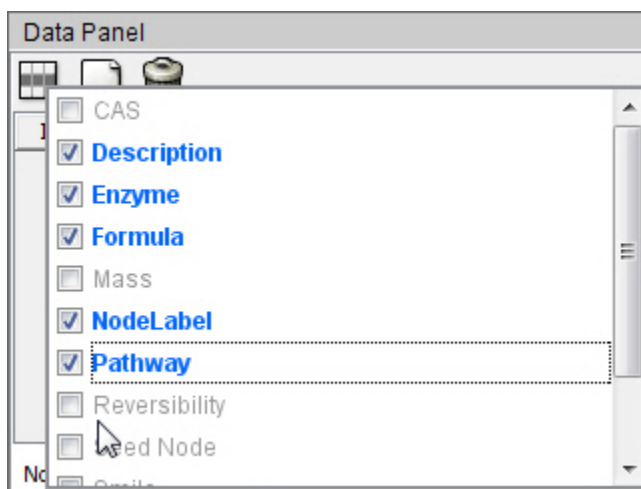
Choosing attributes provided through MetScape

To choose which attributes to view:

- To choose attributes for compounds, click the **Node Attribute Browser** tab in the Data Panel. Choose attributes for reactions based on the network style:
 - If the style is Show Reactions as Nodes, click the **Node Attribute Browser** tab.
 - If the style is Show Reactions as Edges, click the **Edge Attribute Browser** tab.
- Click the **Select Attributes** icon in the Data Panel toolbar.



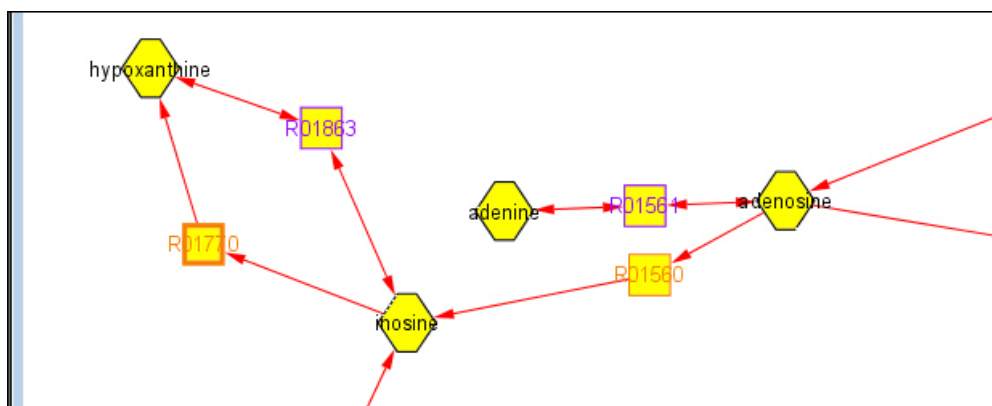
- Select the attributes you want displayed in the Data Panel.



Notes:

- When both compounds and reactions are shown as nodes, you can use the **Type** attribute on the **Node Attribute Browser** tab to distinguish between them.

- Some attributes (such as Formula, Mass, and Smile) apply only to compound nodes, while others (such as Enzyme, Pathway, and Reversibility) apply only to reaction nodes.
 - [Switching from one network style to another](#) using **Show Reactions as Nodes** or **Show Reactions as Edges** may leave behind reaction attribute columns on either the **Node Attribute Browser** or **Edge Attribute Browser** tab.
 - Other plugins used earlier in your Cytoscape session may leave behind attributes that don't apply to MetScape compound or reaction data.
4. When you are done, click anywhere outside the list.
 5. Select compounds and/or reactions to view their attributes in the Data Panel (see ["Selecting Compounds and Reactions"](#)).



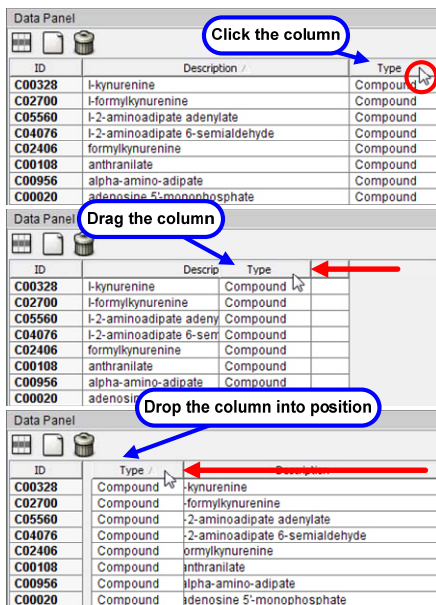
The diagram shows a network of four yellow hexagonal nodes: hypoxanthine, adenine, adenosine, and inosine. Red arrows represent reactions: R01770 (hypoxanthine to inosine), R01863 (inosine to hypoxanthine), R01561 (adenosine to adenine), and R01560 (adenosine to inosine).

Data Panel				
ID	Type	Description ▾	Formula	
R05196	Reaction	(1,4-alpha-D-Glucosyl)n+n Glucose=n Maltose		R051
C00277	Compound	(1,4-alpha-d-glucosyl)n	HO(C6H10O5)n	(1,4-
R00183	Reaction	AMP+H2O=Adenosine+Orthophosphate		R001
R00185	Reaction	ATP+Adenosine=ADP+AMP		R001
R01560	Reaction	Adenosine+H2O=Inosine+NH3		R015
R01561	Reaction	Adenosine+Orthophosphate=Adenine+alpha-D-Ri...		R015
R01770	Reaction	Inosine+H2O=Hypoxanthine+D-Ribose		R017
R01863	Reaction	Inosine+Orthophosphate=Hypoxanthine+alpha-D-...		R018
C00147	Compound	adenine	C5H5N5	aden

Node Attribute Browser | **Edge Attribute Browser** | Network Attribute Browser

Rearranging attributes in the Data Panel

To reorder attributes in the Data Panel, click an attribute column heading and drag it to a new location:



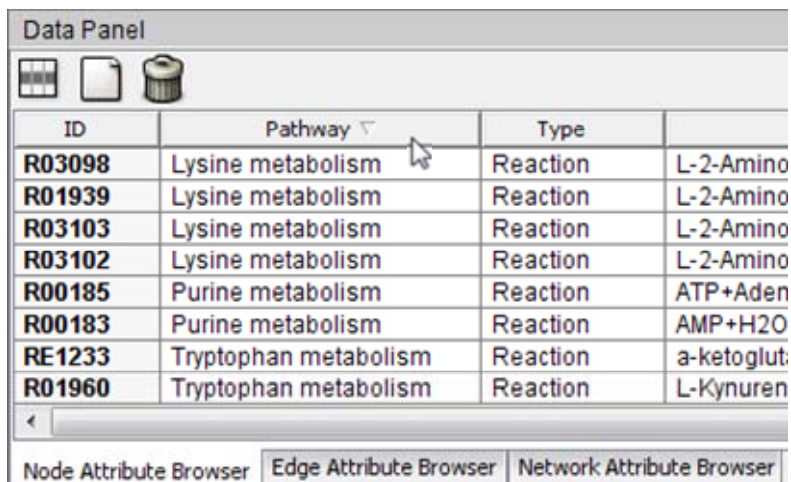
The figure consists of three sequential screenshots of the Data Panel interface, illustrating the steps to rearrange columns:

- Click the column:** The 'Type' column heading is selected with a mouse cursor. A red circle highlights the cursor on the heading.
- Drag the column:** The 'Type' column heading is being dragged from its original position to the left, towards the 'ID' column position. A red arrow indicates the direction of the drag.
- Drop the column into position:** The 'Type' column heading is dropped into its new position to the left of the 'ID' column. A red arrow points to the new position.

The data table in all screenshots is as follows:

ID	Description	Type
C00328	L-kynurenine	Compound
C02700	L-formylkynurenine	Compound
C05560	L-2-aminoadipate adenylate	Compound
C04076	L-2-aminoadipate 6-semialdehyde	Compound
C02406	formylkynurenine	Compound
C00108	anthranilate	Compound
C00956	alpha-amino-adipate	Compound
C00020	adenosine 5'-monophosphate	Compound

To sort by an attribute, click the attribute column heading; to sort in the reverse direction, click again.



The screenshot shows the Data Panel with the following table:

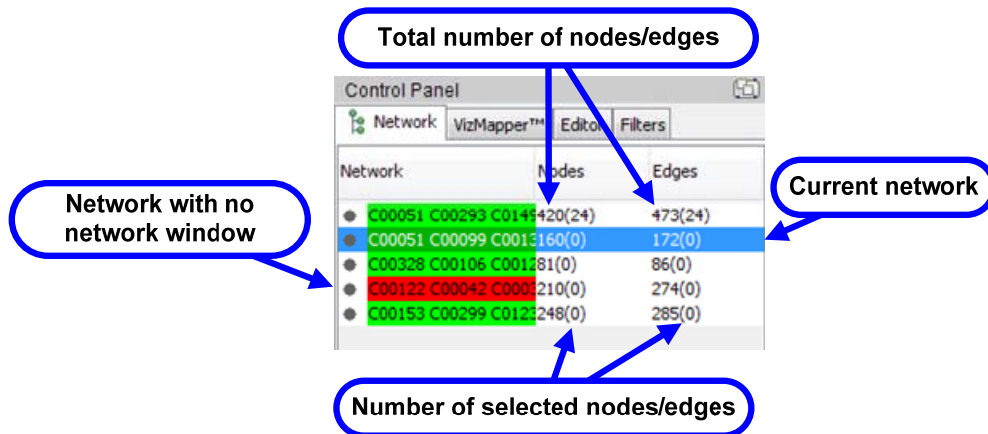
ID	Pathway	Type	
R03098	Lysine metabolism	Reaction	L-2-Amino
R01939	Lysine metabolism	Reaction	L-2-Amino
R03103	Lysine metabolism	Reaction	L-2-Amino
R03102	Lysine metabolism	Reaction	L-2-Amino
R00185	Purine metabolism	Reaction	ATP+Aden
R00183	Purine metabolism	Reaction	AMP+H2O
RE1233	Tryptophan metabolism	Reaction	a-ketoglut:
R01960	Tryptophan metabolism	Reaction	L-Kynuren

At the bottom of the panel, there are three tabs: Node Attribute Browser, Edge Attribute Browser, and Network Attribute Browser.

NAVIGATING A NETWORK

Navigating among networks

To navigate among multiple open networks, use the **Network** tab in the Cytoscape Control Panel.



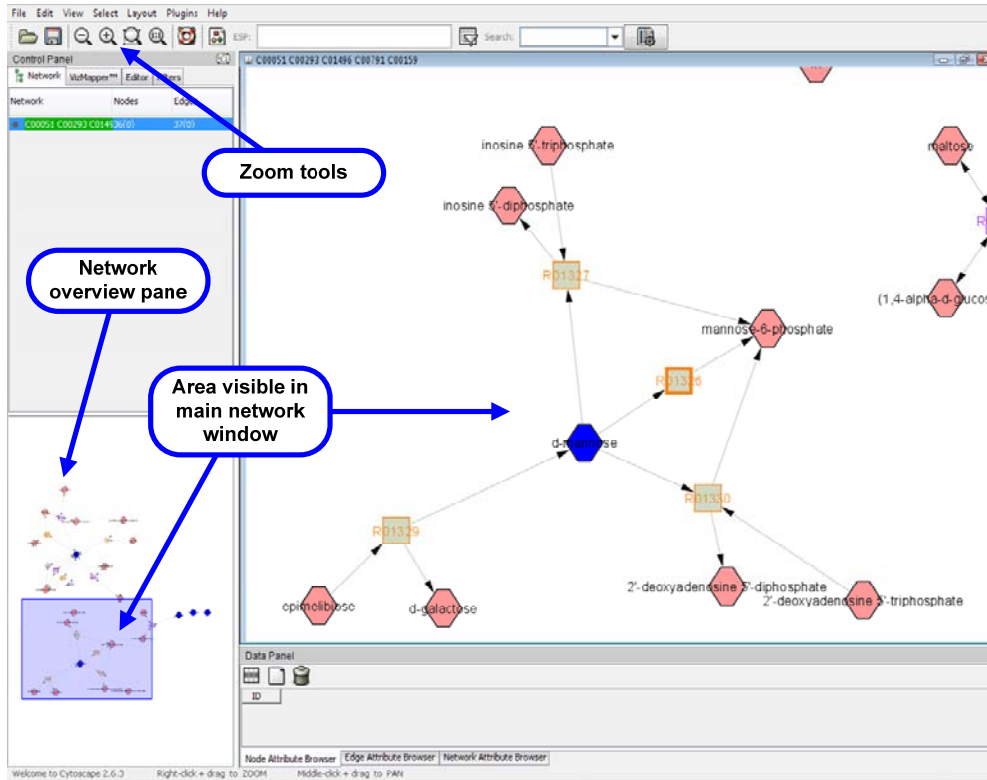
To view a network, click on its entry on the **Network** tab.

Note: The default network title is a list of its initial seed compounds. To edit a title, right-click the network entry and select **Edit Network Title**.

For more information about working with networks and the **Network** tab, see the *Cytoscape User Manual*.





Navigating within a network

To navigate within a network, use the network overview pane at the bottom of the **Network** tab in the Cytoscape Control Panel.



To view another part of the network, click on the shaded area in the network overview pane and drag it into place.

To adjust the view magnification, use the Zoom tools in the Cytoscape toolbar:

- **Zoom Out**  and **Zoom In** .
- **Zoom Selected Region** . Make one or more selections using any Cytoscape method, then click this tool to display the region that encompasses all of them.
- **Zoom Entire Network** .

For more information about zooming and using the network overview pane, see the *Cytoscape User Manual*.

Locating compounds or reactions within a network by searching

You can locate and select a specific compound or reaction within a network by using the Search feature of Cytoscape. You can also use search to find a group of compounds or reactions with common attribute values. Search is especially useful with large, complex networks.

Limitations of the Search feature in Cytoscape:

- For a successful match, the search term must match the entire attribute value. For example, the following Enzyme attributes do not match:
 - 2.3.1.65 [Bile acid-CoA: amino acid N-acyltransferase.]
 - 2.3.1.65 [Bile acid-CoA: amino acid N-acyltransferase.]; 6.2.1.- [Acid--thiol ligases.]
- For a successful match, the search term must match the attribute value from the start of the string—you cannot match a substring within an attribute value. For example, the search term **taurine** matches the first attribute value below, but not the second:
 - taurine+deoxycholoyl-CoA = CoA+H('+)+3"a",12"a"-dihydroxy-5"b"-cholan-24-oyl-**taurine**
 - (5-L-Glutamyl)-peptide+Taurine=Peptide+5-Glutamyl-**taurine**
- Search does not support logical operators, wildcards, or other advanced search features.

Note: For more flexible and powerful searching, including logical operators and wildcards, you can use the Enhanced Search plugin for Cytoscape. For more information, see the Analysis group of plugins on the [Cytoscape Plugins page](#).

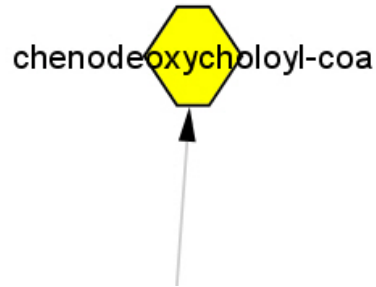
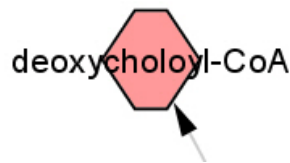
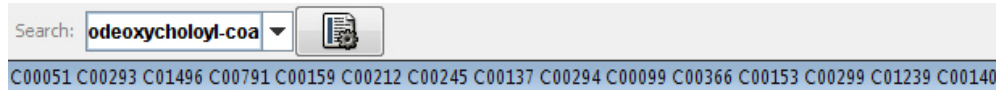
To search for compounds or reactions:



1. Click  (**Configure search options**) to the right of the Search box in the Cytoscape toolbar.

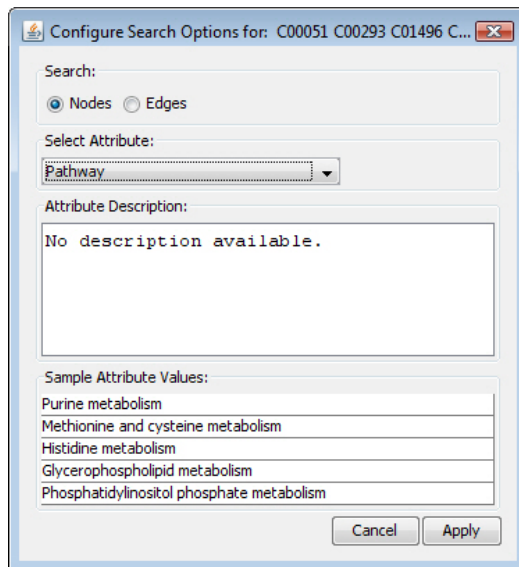
- Select an item in the list to locate the node or edge. Cytoscape zooms to the item and selects it.

Note: Using Search to select a reaction shown as an edge also selects the connected compounds; selecting a reaction shown as a node does not.

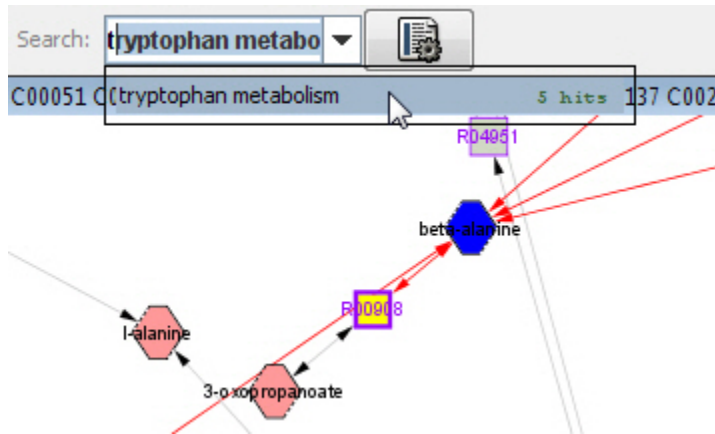


Example: Locating reactions on the same pathway (tryptophan metabolism)

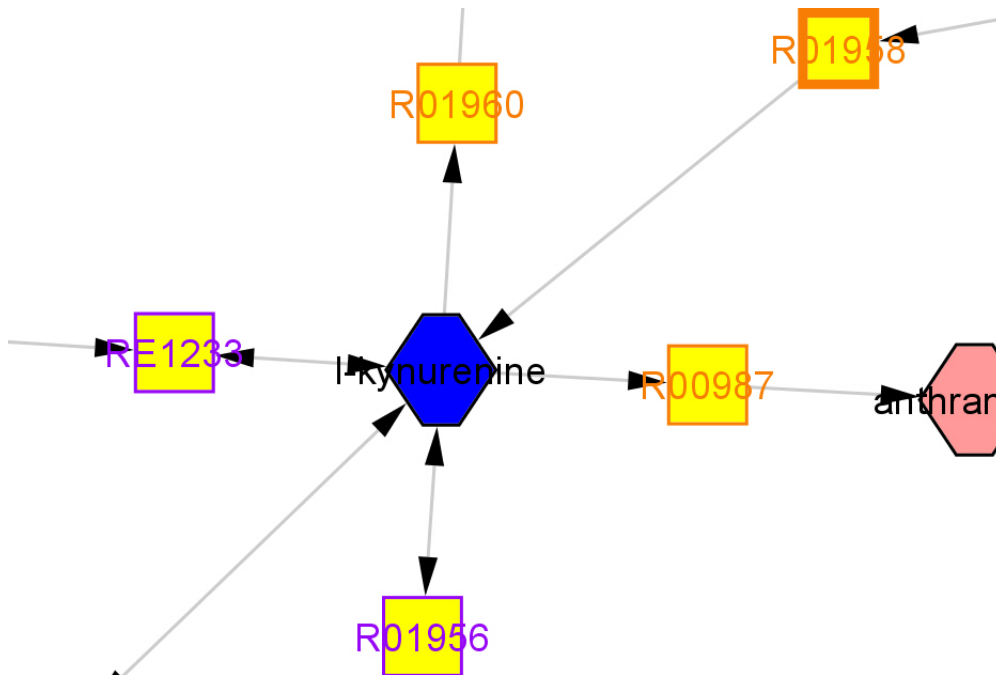
- Select the **Pathway** attribute for reactions (in this example, shown as nodes).



- Type in the **Search** box, select **Tryptophan metabolism** (with 5 matching reactions), and press **Enter**.



- The 5 reactions are selected.



4. The Data Panel displays attributes for the selected reactions.

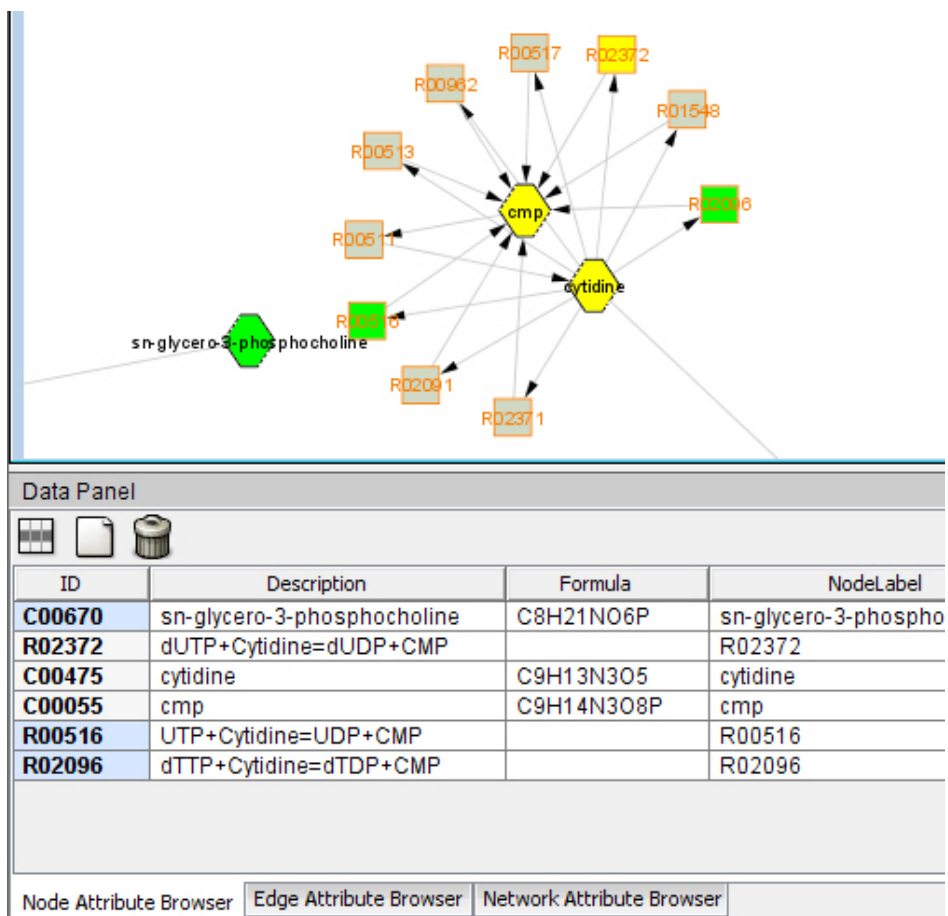
Data Panel			
ID	Pathway	NodeLabel	Description
R01958	Tryptophan metabolism	R01958	Formylkynurenine+H2O=Fi
R01960	Tryptophan metabolism	R01960	L-Kynurenine+Oxygen+NAI
R00987	Tryptophan metabolism	R00987	L-Kynurenine+H2O=Anthra
RE1233	Tryptophan metabolism	RE1233	a-ketoglutarate+L-kynureni
R01956	Tryptophan metabolism	R01956	L-Kynurenine+2-Oxoglutar:

Locating compounds or reactions using the Data Panel

You can locate compounds and reactions in the network by selecting their attributes in the Data Panel.

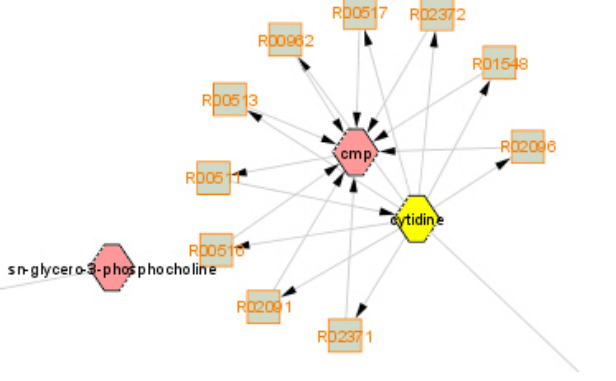
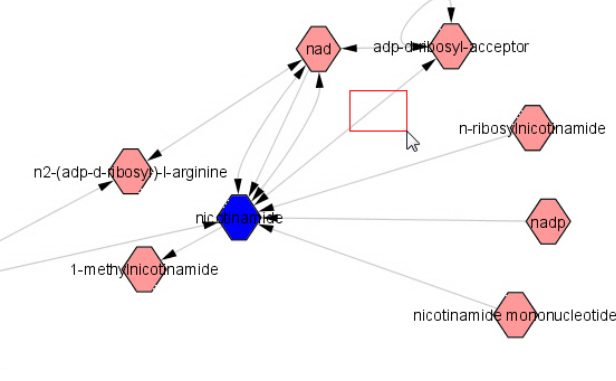
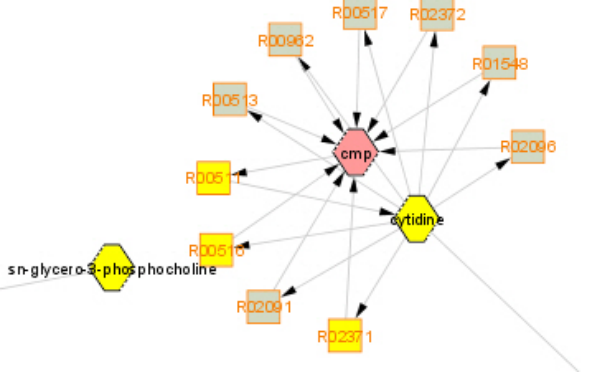
1. Click the **Node Attribute Browser** or **Edge Attribute Browser** tab in the Data Panel.
2. Select attribute rows for the nodes or edges you want to locate.
 - Click on a single row to highlight a single compound or reaction.
 - Use Ctrl-click to select multiple discontinuous rows.
 - Use Shift-click to select a range of contiguous rows.

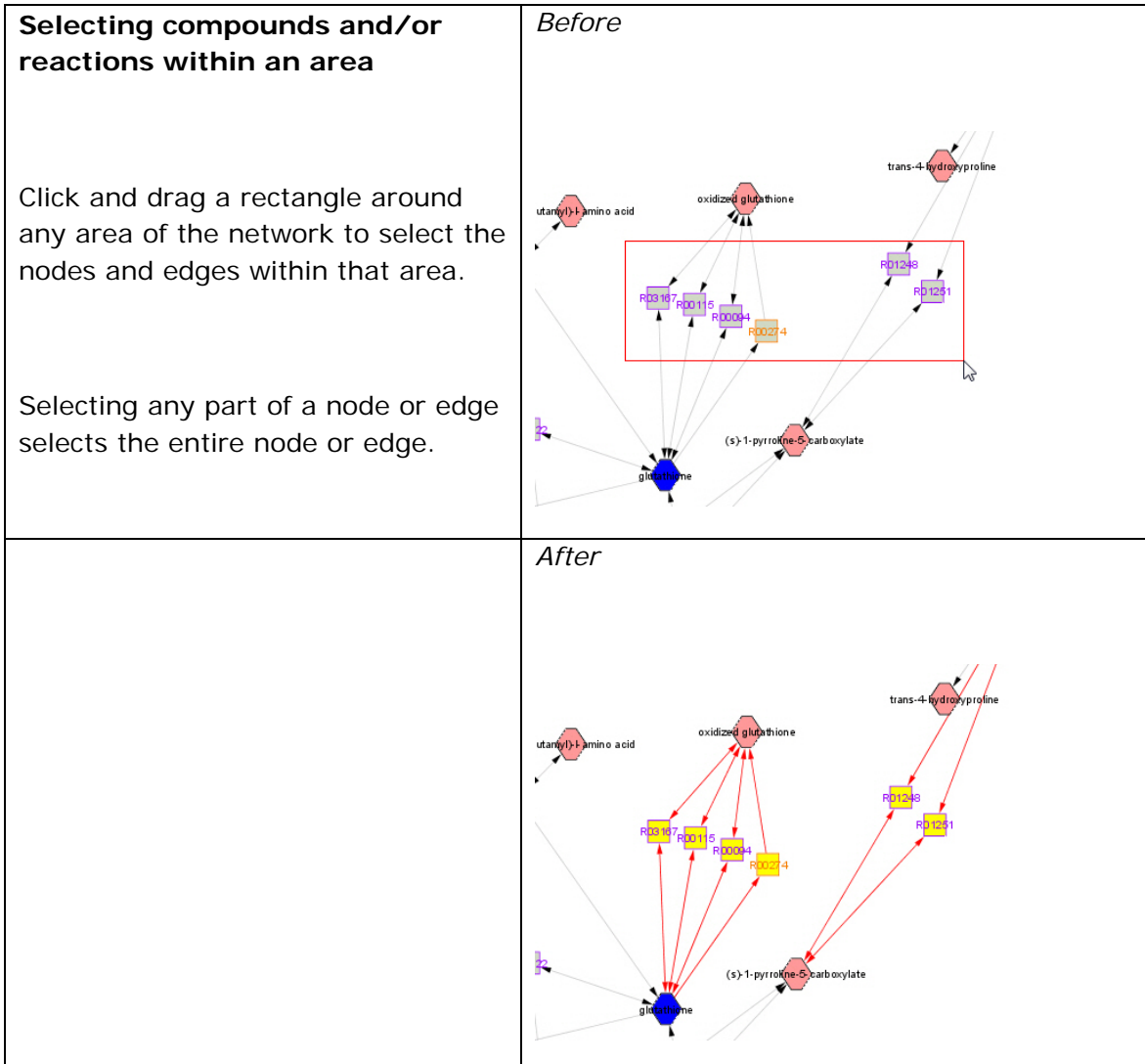
3. For selected rows, the corresponding compounds and/or reactions are highlighted in green in the network view. (See "[Selecting Compounds and Reactions.](#)")



SELECTING COMPOUNDS AND REACTIONS

Use Cytoscape methods to select nodes representing compounds and reactions (when shown as nodes) and edges representing reactions (when shown as edges).

<p>Selecting a single compound or reaction shown as a node</p> <p>Click the compound or reaction node.</p> <p>A selected node appears in yellow.</p>	
<p>Selecting a single reaction shown as an edge</p> <p>Click and drag a rectangle around any segment of the reaction edge, then release the left mouse button.</p> <p>A selected edge appears in red.</p>	
<p>Selecting multiple compounds and/or reactions</p> <p>Hold down the Shift key while clicking on nodes and/or edges and/or while dragging rectangles around them.</p>	



For more information

For detailed information on selecting nodes and edges in a network, see the *Cytoscape User Manual*.

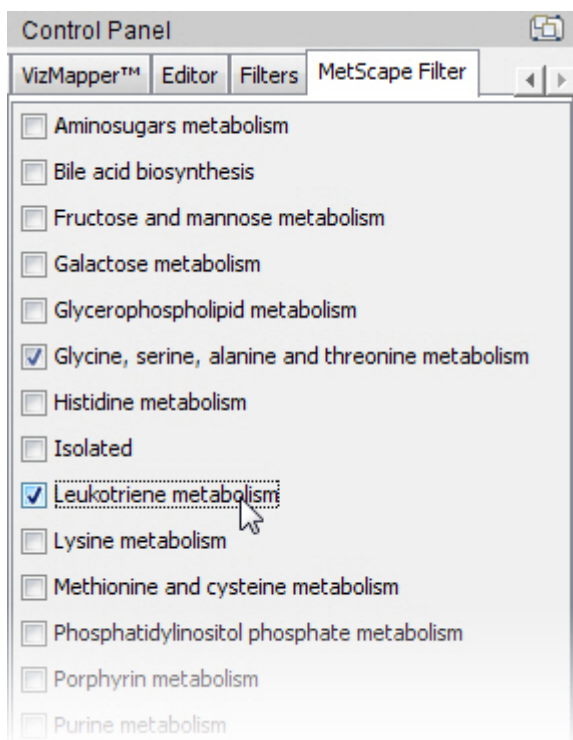
FILTERING REACTIONS BY PATHWAY

You can highlight reactions associated with specific pathways, and optionally create a subnetwork containing only those reactions.

Note: Pathway filtering works only when reactions are shown as nodes.

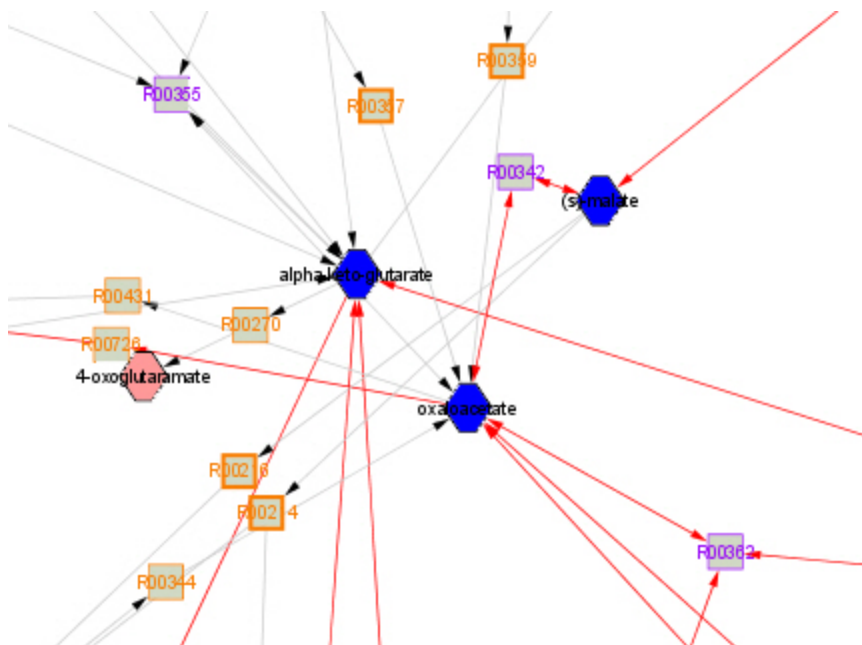
To filter reactions by pathway:

1. Right-click on any node (compound or reaction).
2. Select **MetScape** → **Pathway Filter** to display the **MetScape Filter** tab in the Cytoscape Control Panel.
3. Select one or more pathways of interest.



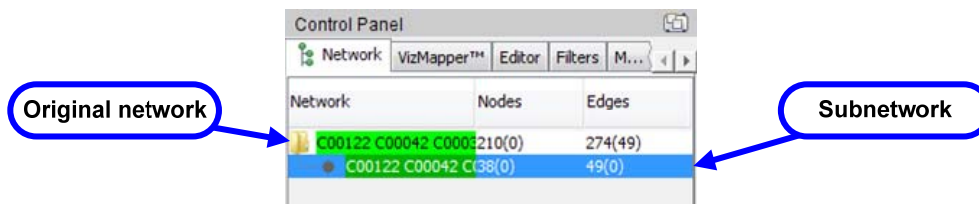
4. Click the **Filter** button at the bottom of the **MetScape Filter** tab to highlight reactions in the network that are in the selected pathways.

All connected edges to matching reactions and compounds are highlighted in red.



- To create a new subnetwork of the original network containing only those reactions in the selected pathways, click the **Create SubNetwork** button.

The subnetwork appears as a child of the original network on the **Network** tab in the Control Panel.



ACCESSING ADDITIONAL COMPOUND AND REACTION INFORMATION

In addition to viewing compound and reaction attribute values for selected nodes in the Cytoscape Data Panel (see "[Choosing Attributes for Display in the Data Panel](#)") and displaying attributes by hovering the mouse cursor (see "[MetScape plugin selection behavior](#)"), you can display additional information and link to external databases.

Displaying compound and reaction details

To display details about a compound or reaction:

- Double-click the compound node, reaction node, or reaction edge.

Details appear on the **Node/Edge Details** tab in the Cytoscape Results Panel.

Details beyond the attributes that appear in the Data Panel include:

Compound details:

Reaction details:

Compound details:

C00322
Compound
Primary Name: 2-oxoadipate
Synonym: 2-oxoadipic acid
Formula: C₆H₈O₅
Mass: 160.0
CAS: 3184-35-8
Smile: C(CC(=O)C(=O)O)CC(=O)O
Links: [MiMI \[C00322\]](#), [KEGG \[C00322\]](#), [PubChem \[71\]](#), [BioCyc \[2K-ADIPATE\]](#), [ChEBI \[15753\]](#), [HMP \[HMDB00225\]](#)
KEGG 2D structure:
OC(=O)CCCC(=O)O
C00322

Reaction details:

R01958
Reaction
Equation: Formylkynurenine+H₂O=Formate+L-Kynurenine
Enzyme: -3.5.1.49 [Formamidase.], -3.5.1.9 [Arylformamidase.], Corresponding genes from MiMI: [125061 \[Symbol: AFMID\]](#)
Pathway: Tryptophan metabolism
Reversible [y/n]? N
Links: [MiMI \[R01958\]](#), [KEGG \[R01958\]](#)

WORKING WITH NETWORKS

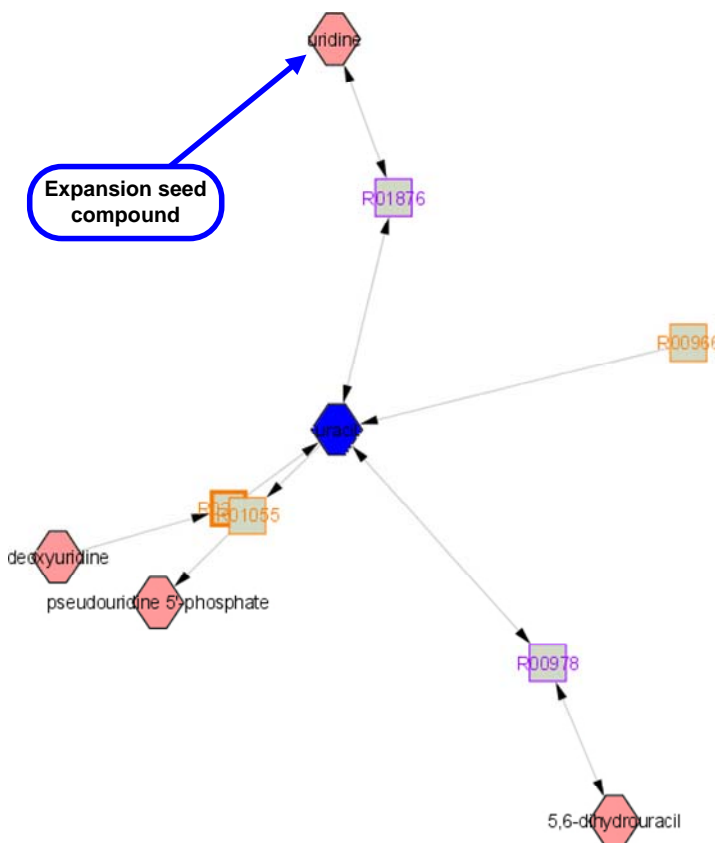
Expanding a network

From a compound node, you can expand the current network to include additional reactions and related compounds.

Option 1: Expanding a network in the current network window

1. Right-click the compound node you want to expand (the *expansion seed compound*).

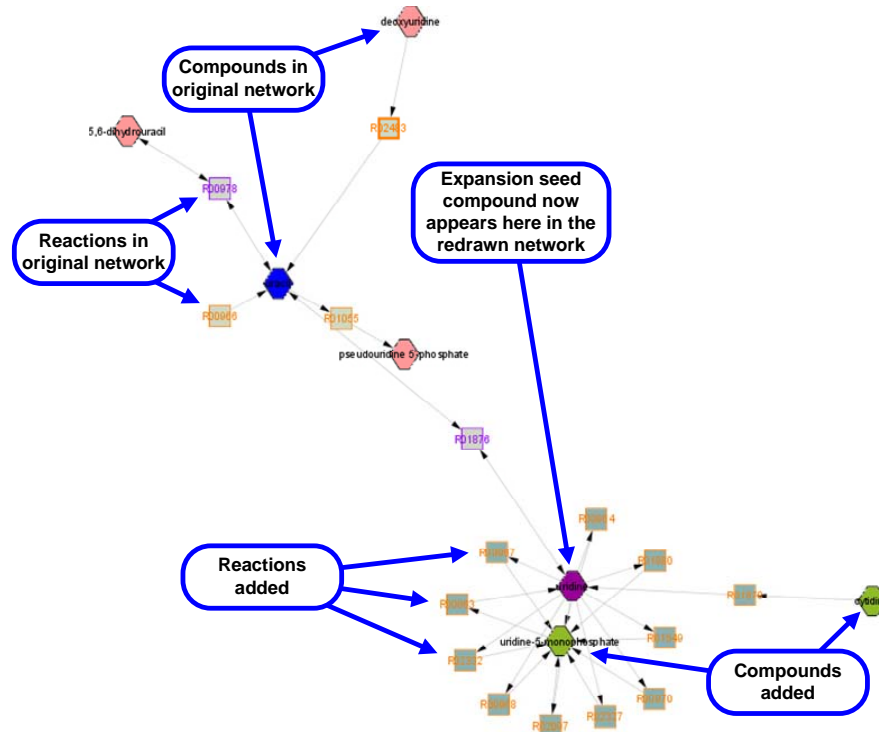
Original network:



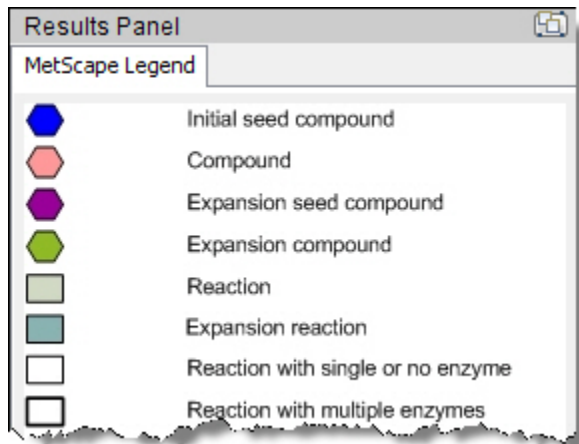
2. Select **MetScope** → **Expand** → **Expand in Current Window**. As a result:
 - The current network view may be redrawn.
 - The expansion seed compound may appear in a different location in the redrawn network view.
 - Additional compounds and reactions are added to the current network.

- On the **Network** tab in the Control Panel, the number of nodes and edges in the network is updated.

Network expanded in the current window:



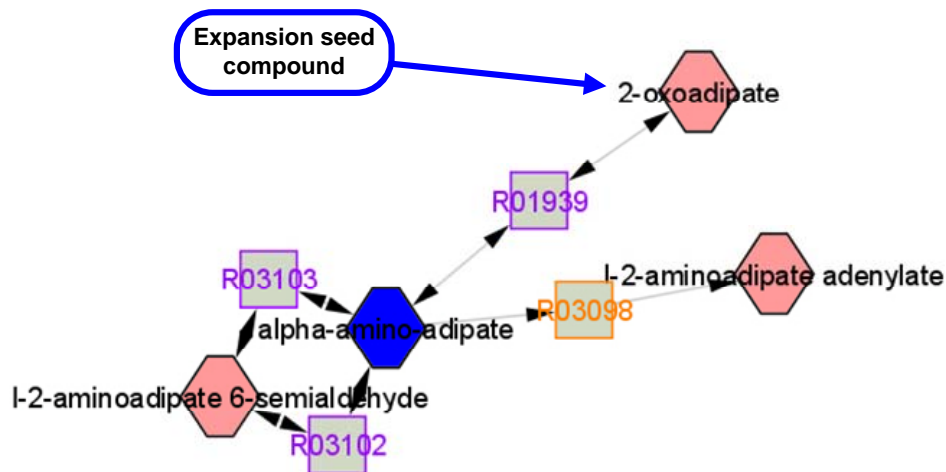
When you expand a network in the current window, the network view includes additional symbols, as shown in the **MetScape Legend**:



Option 2: Expanding a network in a new window

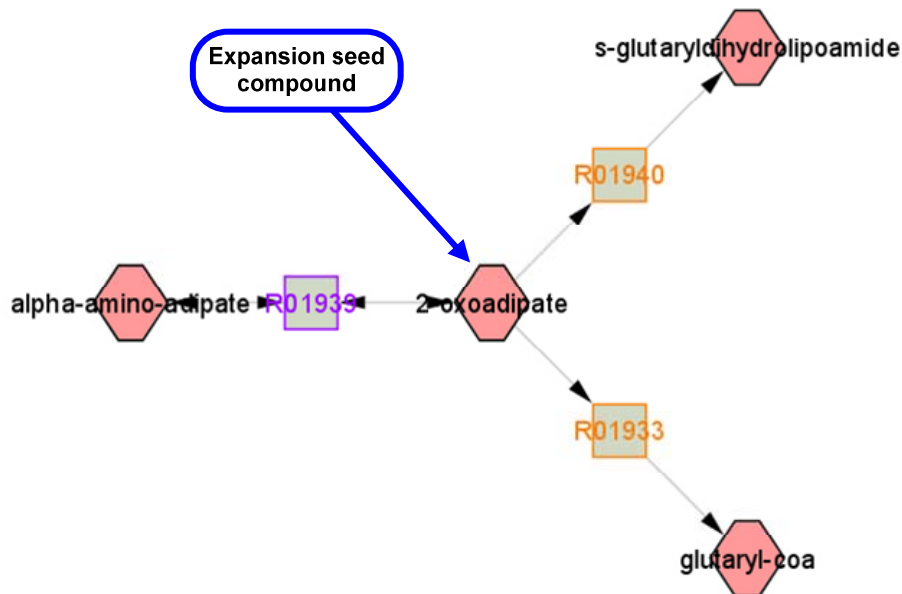
1. Right-click the compound node you want to expand (the expansion seed compound).

Original network:




2. Select **MetScape** → **Expand** → **Expand in New Window**. As a result:
 - A new network is created in a new network view window.
 - The new network includes only the expansion seed compound and its related compounds and reactions.
 - Nodes and edges appear using standard symbols, not expansion symbols.
 - On the **Network** tab in the Control Panel, a new network entry is created. The default network title is the compound ID of the expansion seed.

Network expanded in a new window:



Collapsing a network

To collapse a network expanded in a current network window:

1. Right-click an expansion seed compound node .
2. Select **MetScape** → **Collapse**, and then:
 - To collapse only the branch expanded from that expansion seed compound, select **Collapse**.
 - To collapse all expanded branches, select **Restore Original Network**.

Creating a subnetwork

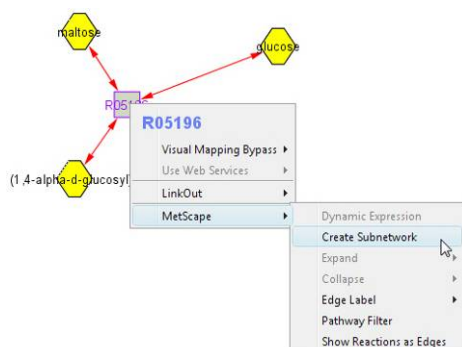
You can create a subnetwork (child network) of the current network that will appear in its own network view:

- A subnetwork based on a compound includes the compound and all reactions in the parent network in which the compound participates.
- A subnetwork based on a reaction includes the reaction and all compounds in the parent network that participate in the reaction.

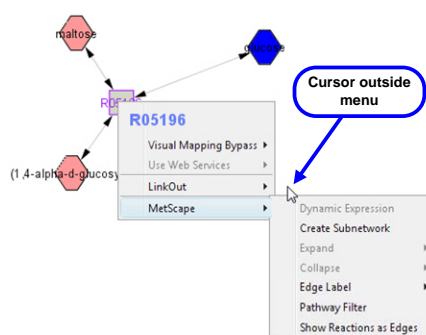
Note: A subnetwork will include any nodes and edges highlighted (nodes in yellow, edges in red) at the time you create the subnetwork. This includes any nodes or edges that are currently selected. If you want a subnetwork based on a single compound or reaction as described above, first clear all selections by clicking any blank area of the network view.

1. In the network view, select the compound or reaction on which you want to base the subnetwork. Nodes highlighted in yellow and edges highlighted in red will become part of the subnetwork.
2. Right-click the node and select **MetScape** → **Create Subnetwork**. Be careful not to move the cursor outside the bounds of the gray menu panels while navigating the cascading menu—doing so will remove the highlighting of the nodes and edges and the result will be an empty subnetwork.

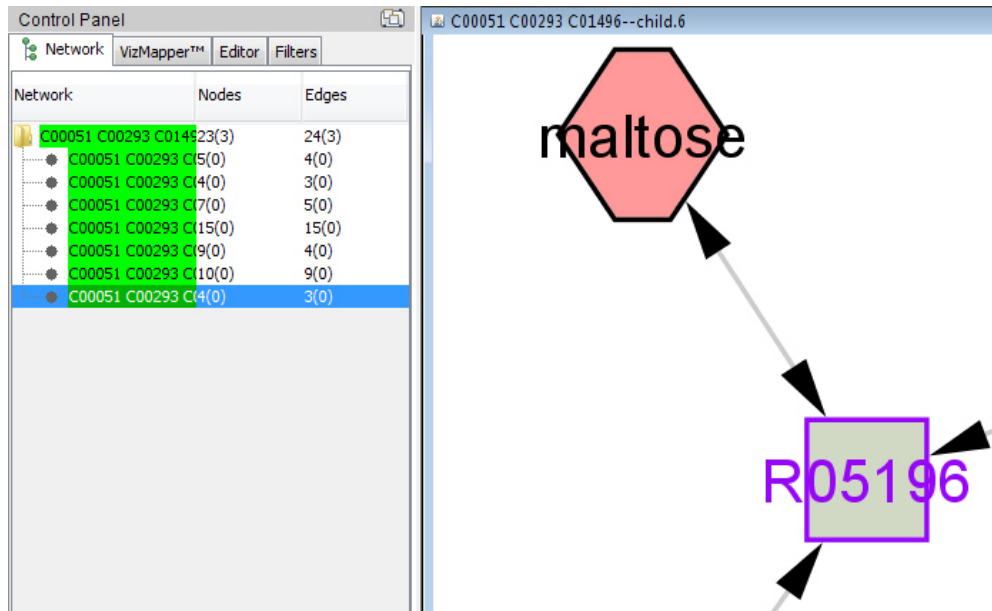
Correct



Incorrect



The newly created subnetwork appears in its own network view window, and is added as a subnetwork (child) of the original (parent) network on the **Network** tab in the Control Panel:



See also "[Filtering Reactions by Pathway](#)" for information on creating a subnetwork from a pathway filter.

Destroying a network

To destroy a network you no longer need:

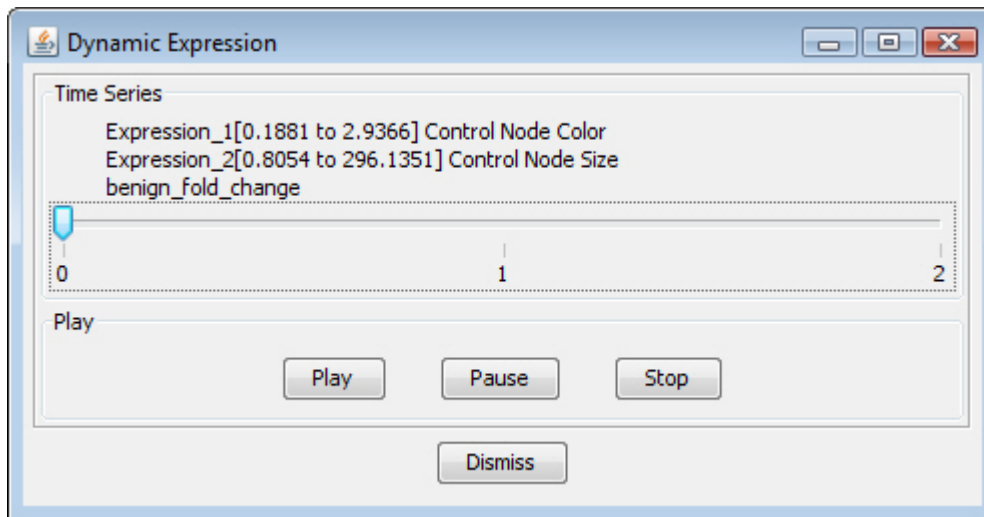
1. Make sure you want to destroy the network:
 - Cytoscape will not ask you to confirm the deletion.
 - Destroying the network is irreversible.
 - **Note:** If you want to destroy a network view without destroying the network itself, use **Destroy View** instead of **Destroy Network**. See the *Cytoscape User Manual* for more information.
2. On the **Network** tab in the Control Panel, right-click on the network you want to destroy (the network does not need to be selected), and select **Destroy Network**.

Note: If you destroy a network that has subnetworks, the subnetworks are *not* destroyed. They are promoted up one network level.

VISUALIZING CHANGES IN EXPERIMENTAL DATA

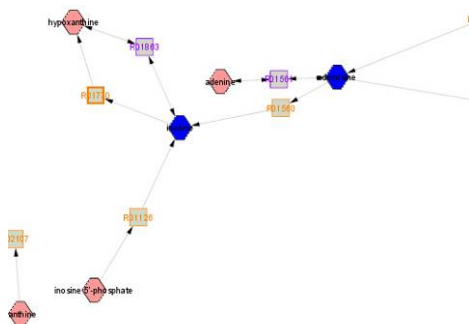
To visualize changes in experimental data:

1. Load a properly formatted experiment file. (See "[Load an experiment file.](#)")
2. Make sure the nodes that are of interest to you are *not* selected. The color changes representing changes in data values will not be visible with the selection color (yellow) applied.
3. Right-click on any node and select **MetScape** → **Dynamic Expression** to display the **Dynamic Expression** dialog:

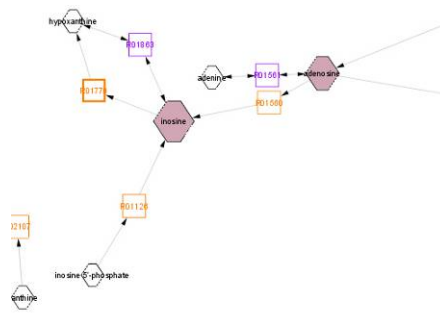


The network display changes to show nodes in variable color and size ranges, based on the values in your experiment file:

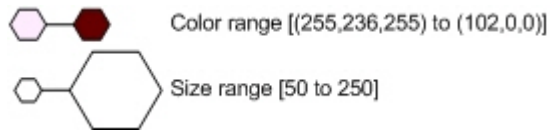
Normal display



Dynamic Expression display



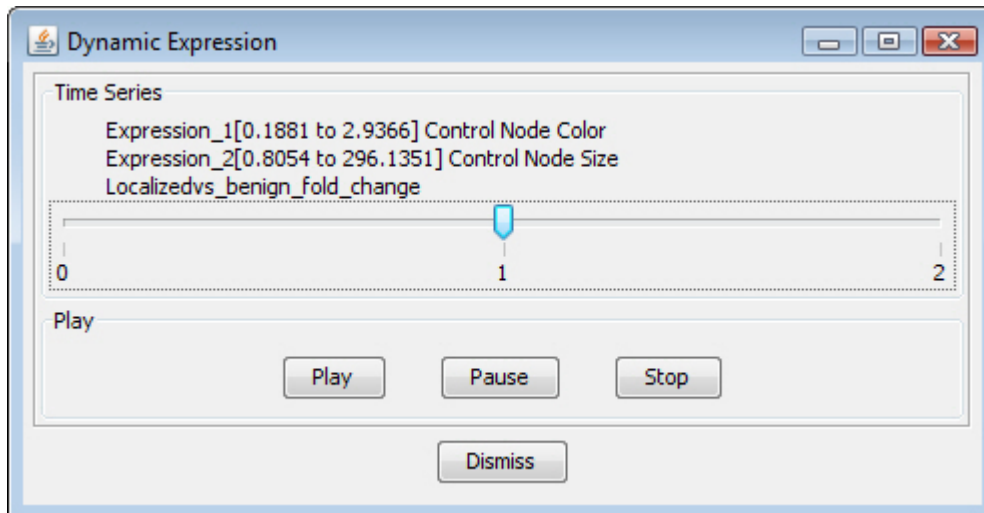
The color and size ranges in the MetScape legend apply to nodes in Dynamic Expression:



The color range shows changes in value for the first parameter in your experiment file, the size range for the second parameter in your experiment file.

- To visualize your experiment file data, you can:

Show values of a particular data set by moving the slider (from **0** to **1** in the following example):



The line of text above the slider also changes to show the current column heading of data from your experiment file.

You can also play an animation using the **Play**, **Pause**, and **Stop** controls in the **Dynamic Expression** dialog. When an animation is playing, the slider in the **Dynamic Expression** dialog moves from point to point, and the network view displays the values at each point, using the appropriate color and size ranges.

- When you are done, click **Dismiss**.

SAVING AND REOPENING A SESSION

Saving a session

To save a Cytoscape session containing one or more MetScape plugin networks:

- Select **File** → **Save** (or **Save As...**) from the Cytoscape menu.
- Browse to a location for the session file.

3. Name the file.
4. Click **Save**.

Reopening a session

To reopen a saved session containing MetScape plugin data:

1. Select **File → Open** from the Cytoscape menu.
2. Navigate to the file location.
3. Select the file.
4. Click **Open**.
5. After Cytoscape reports that the session file was successfully loaded, click **Close**.

USING METSCAPE PLUGIN-SPECIFIC FEATURES IN CYTOSCAPE

Switching network style for showing reactions

You can switch from showing reactions as nodes to showing them as edges, or vice versa.

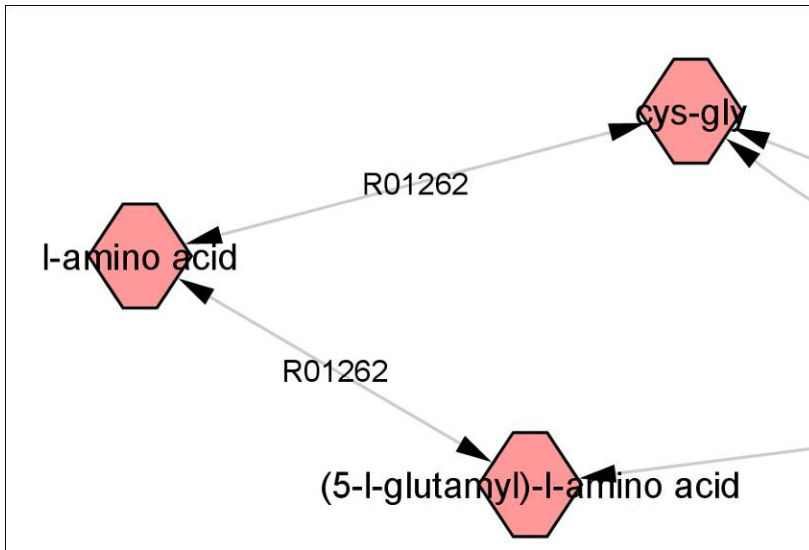
1. Right-click on any node.
2. Select **MetScape → Show Reactions as Nodes** or **Show Reactions as Edges**.

The network view is redrawn in the selected style. Switching network style also affects the attributes available in the **Node Attribute Browser** and **Edge Attribute Browser**.

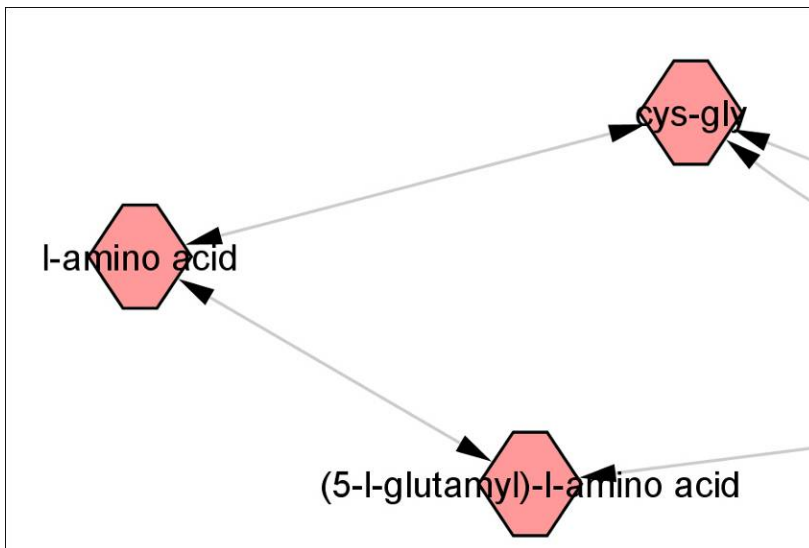
Labeling reactions shown as edges

When reactions are shown as edges in the network view, you can display their reaction IDs to identify them.

1. Right-click on any node.
2. Select **MetScape → Edge Label → Show Edge Label**.



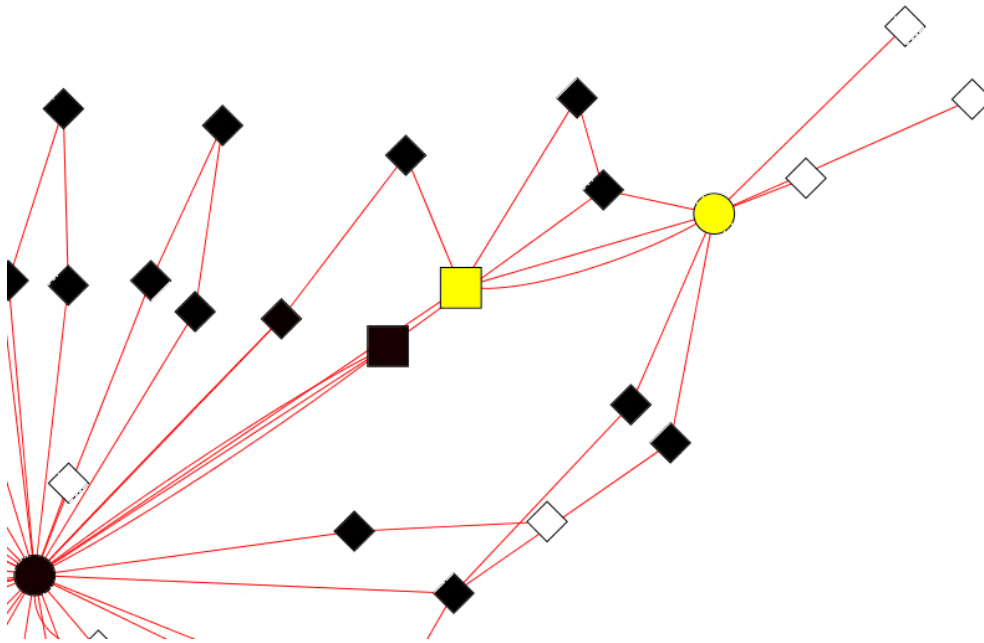
3. To hide the IDs, select **Hide Edge Label** instead.




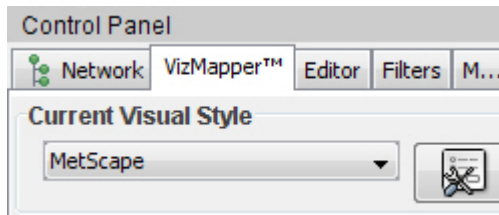
Restoring the MetScape visual style

You may need to restore the MetScape visual style after using a different plugin that uses its own style.

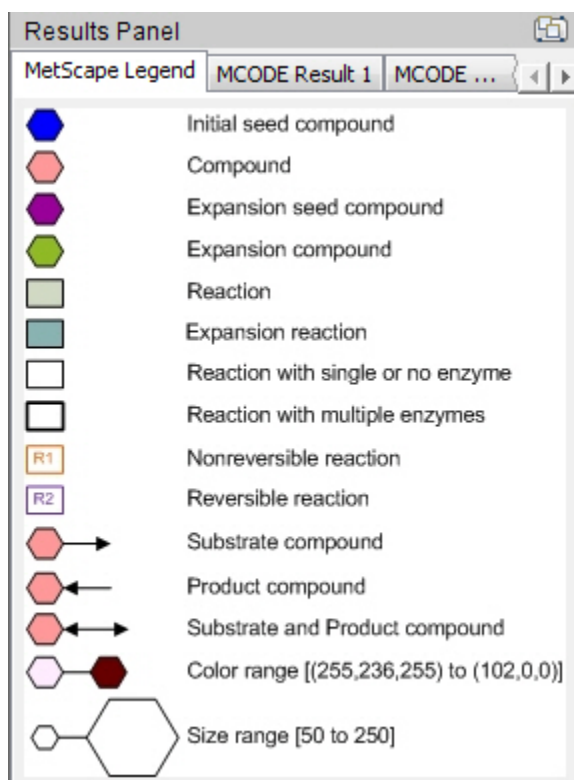
Network after using the MCODE plugin with MCODE visual style



1. In the Cytoscape Control Panel, click the **VizMapper™** tab. You may need to use the scroll arrows   at the top of the Control Panel to see the tab.
2. For **Current Visual Style**, select **MetScape**:



3. The MetScape visual style is restored:



- Reaction symbols in the legend apply to reactions when shown as nodes.
- Color and size range symbols apply to Dynamic Expression displays (see [“Visualizing Changes in Experimental Data”](#)).

Note: If you open a saved Cytoscape session, the **MetScape Legend** tab does not appear in the Results Panel until you use the MetScape plugin to [enter data](#) in a new query.