projectName Documentation

project version

developerList

timestamp

Abstract

1 Introduction

EnrichedChem Plugin for Cytoscape is a chemical tool for visualizing compound similarity in the Cytoscape environment. It supports results from different data processing programs like Hierarchical Clustering, CMAP and etc. It can search matched compound from PubChem based on compound name; calculate compound similarity; connect all compounds according to their similarities and show out by a network. It provides an easy to use one-key compound search function searches compound information from Pubchem. The plugin can also be connected to a Mongo DB database as stream to accelerate all processes.

Compared to a plugin in Cytoscape app market named ChemViz with similar functions, EnrichedChem has a better function in searching matched compounds through name, and provides some features ChemViz doesn't have. EnrichedChem also supports using them together to get more powerful results.

2 Instruction

2.1 Control Panel

As Figure 1 shows, the main panel contains a few buttons.

One is load button with which you can load data from certain files. Another is search button which helps you search compounds from Pubchem. And a "drawEdges" button which calculates compound similarity and organizes all nodes to a network.

You can simply change the edge-width-cut-off value with a slider. The two compounds whose similarity is smaller than the value will not be connected. The nodes on the network are organized by their links.

There is a scroll view shows all the information during process. Yellow texts mean warning and red means error.

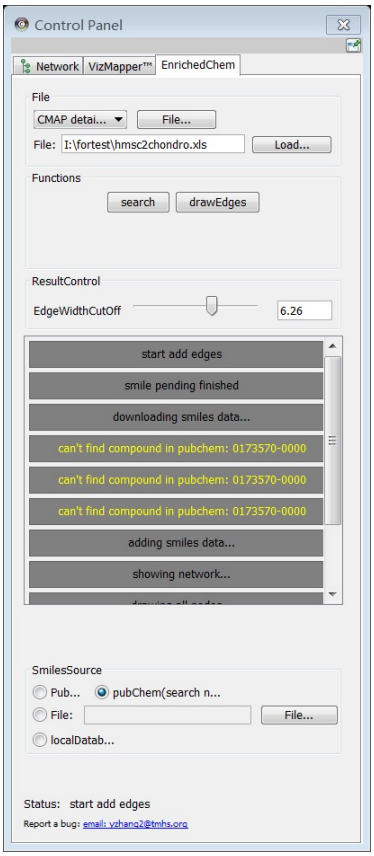

Figure 1: controlPanel

2.2 Load File

EnrichedChem only supports CMAP detailed result file right now. Click File to browse to the file and click load to load the file.

2.3 Search Function

After CMAP detailed results are loaded. Click this button to search for matched compounds from PubChem library. Be sure to have an Internet access, or the plugin wont work. One thing you should remember is that the plugin only searches for the compounds you selected. If you want to search all the compounds, you should leave nothing selected. The search results will be shown on the search result panel which is on the bottom of the screen (Figure 2).

In the middle of the search result panel, all compounds are listed. Every name has some possible matched compound listed below. Every cell on the table is a compound. Click on the cell will show the compounds structure and

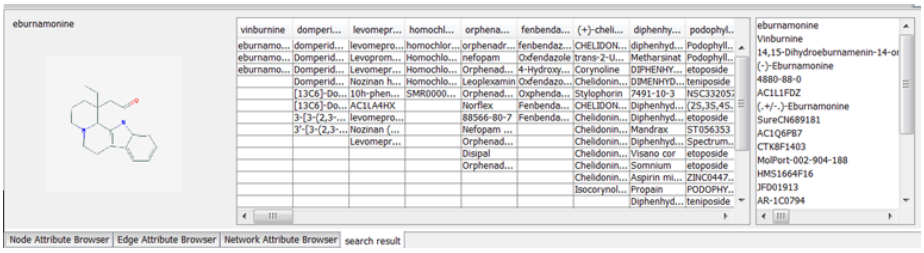

Figure 2: search results panel

name on left and its possible names (alias) on right. We select the first, at the top of the table, as the default best match. If you want other possible result to be the best match, just double click on the table cell. The compound will be up to first and the nodes attributes will be changed.

If some compound on the table dont have results or none of the results matched well. You can try to modify the name of the compound on the Node Attribute Brower panel. And select the changed node click search again. The system will just search for compounds you selected.

2.4 Draw Edges Function

If you are satisfied with all the results, you can continue with the draw edge process. All you need to do is clicking the Draw Edges button.

2.5 Edge Width Cut Off

3 The Network

The network contains a few graphic elements to indicate different values. For different file types, the definition is various. Please refer to certain file instructions below.

But for all file types, the edges widths indicate the similarity between the compounds.

3.1 CMAP Detailed Results^{Figure3}

Here is the define of the graph elements.

Nodes size: the absolute value of score. If the size is bigger, the compound will be more effective.

Color: Red indicates negative value and green indicates positive value.

Pie Chart: The Chart has two parts corresponds to the up and down value.

[1]This image is from cytoscape 2.x, needs to be updated.

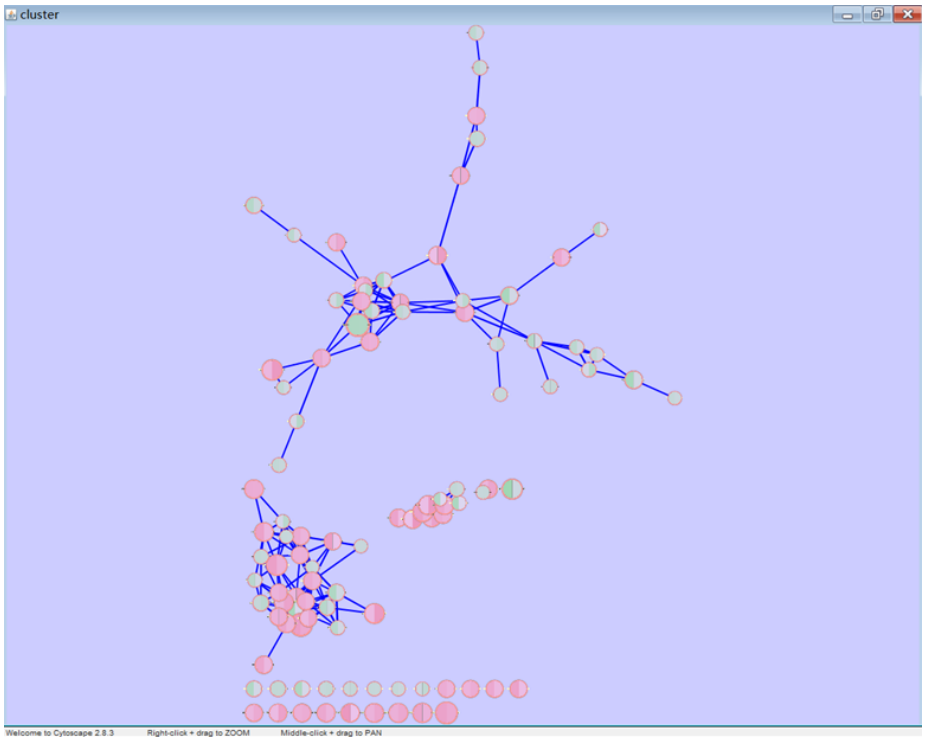

Figure 3: the CMAP network[1]

4 Release Updates

4.1 Version - 1.4-alpha

1.x version is capable with Cytoscape 2.x. But as for some reason, the mutithread process sometimes block the whole Cytoscape environment. This version will not be released until this bug is fixed.

And this version is made a brunch for developing the Cytoscape 2.x version.

4.2 Version - 2.3.x

Version 2.3.0 is a first usable version for cytoscape 3.x. Some bugs may apply to this version. Like:

1. When select nodes, the selected node can't be highlighted.

This version can be release soon because there is no crashing bug. And is stable according to some test.

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