CCCExplorer

v1.1.0

Contents

1. Installing CCCExplorer on Windows

Install JRE

CCCExplorer is a java based application. So the user needs to install JRE before using it.

The user can download JRE package from the link below.

http://www.oracle.com/technetwork/java/javase/downloads/jre7-downloads-1880261.html

Install R language and dependent packages

Download R language for Windows from http://cran.rstudio.com/

https://cran.r-project.org/bin/windows/base/

Install R 3.2-0 or upper version

Open RGui to install following packages.

```
>install.packages("igraph")
```

Run CCCExplorer

Decompress CCCExplorer_v1.1.0.zip

1. Double click "run.batCCCExplorer.jar" to run it.
    1. If you are using Linux or MacOS, run "./run.sh" command in your Terminal.
2. Click "setting" icon, there is a popup dialog. Click "Browse" button to find the Rscript.exe file.
3. After setting the path of Rscript.exe, you can select the files of source and target cell expressions to run your project.

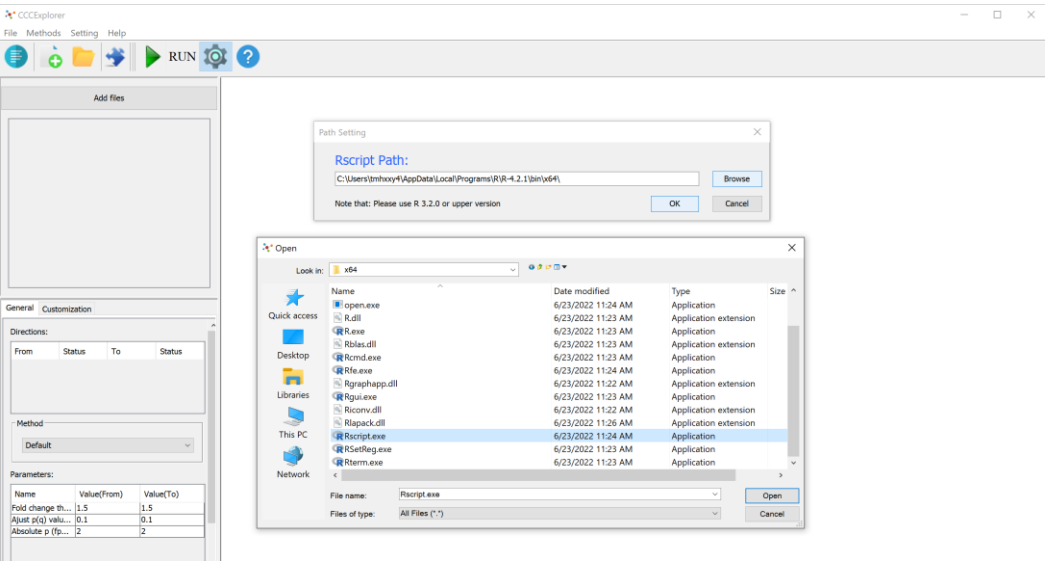**Formatted:** Indent: Left: 0.5", No bullets or numbering

Figure 1

2. How to use CCCExplorer

2.1 Run a project

To run a project, first of all, user needs to select the input files, configure some parameters and choose the specific algorithm program.

~~User can load the input file from the remote server or local disk~~User can add multiple cell type files by clicking "Add Files" button, eg. Figure 2. Then select directions like~~,~~ Figure 3.
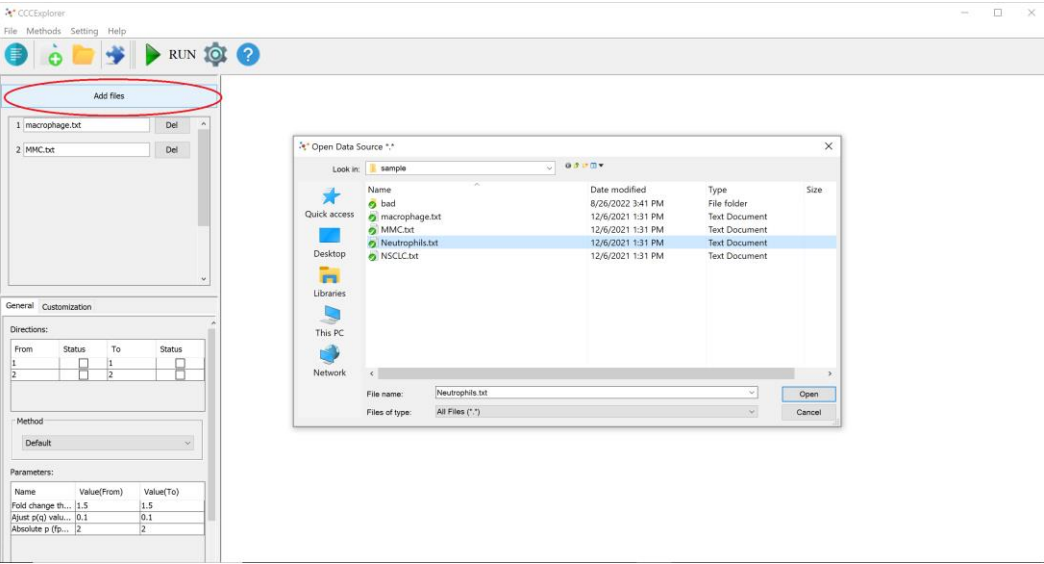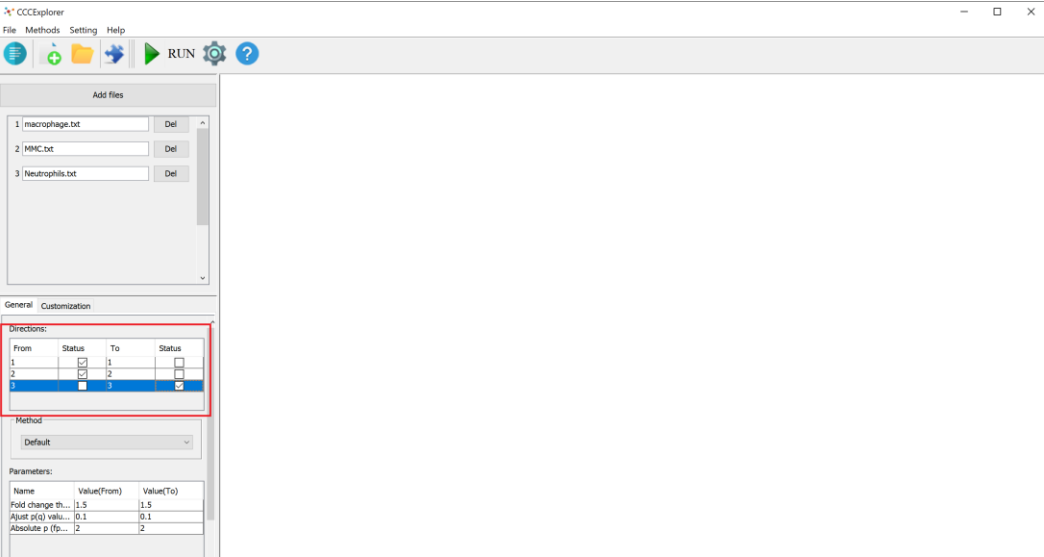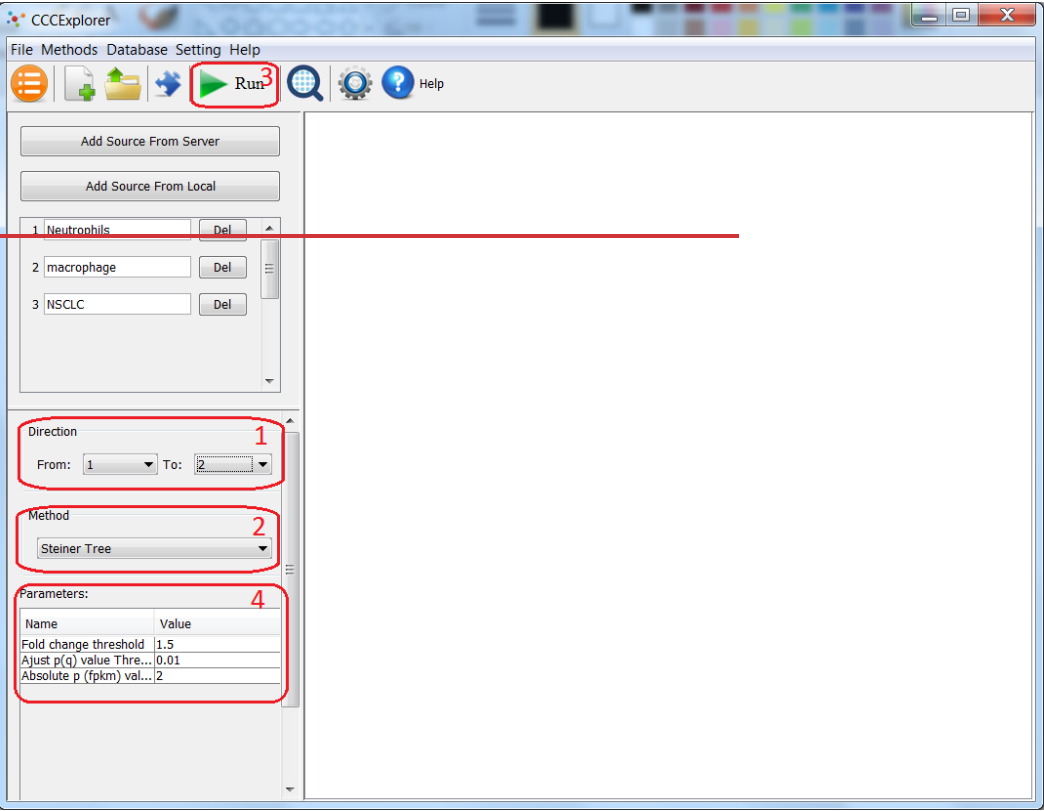
Figure 2

Figure 3

~~User needs to load at least two input files into CCCExplorer. And then selects the direction in box 1, selects the algorithm program in box 2 and set the parameters in box 4.~~ Clicks on "Run" button to run this project. Eg. Figure 4.
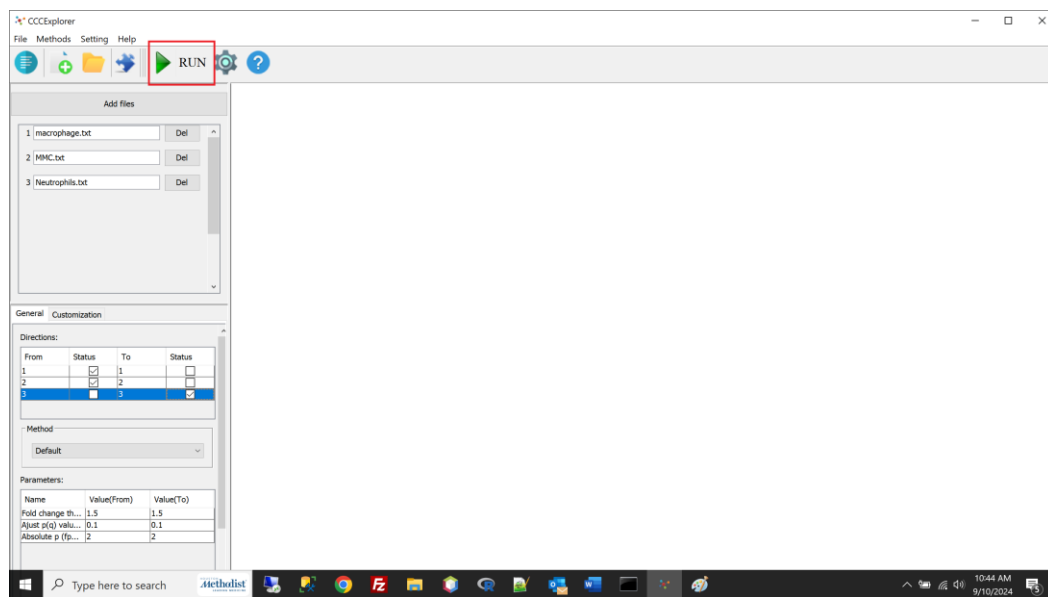
Figure 4

Check the result of a project

When the project is ~~ran~~run successfully, there is an ~~output~~ overview window will show up as Figure 5. Click the pathways you can open the view of the specific direction.
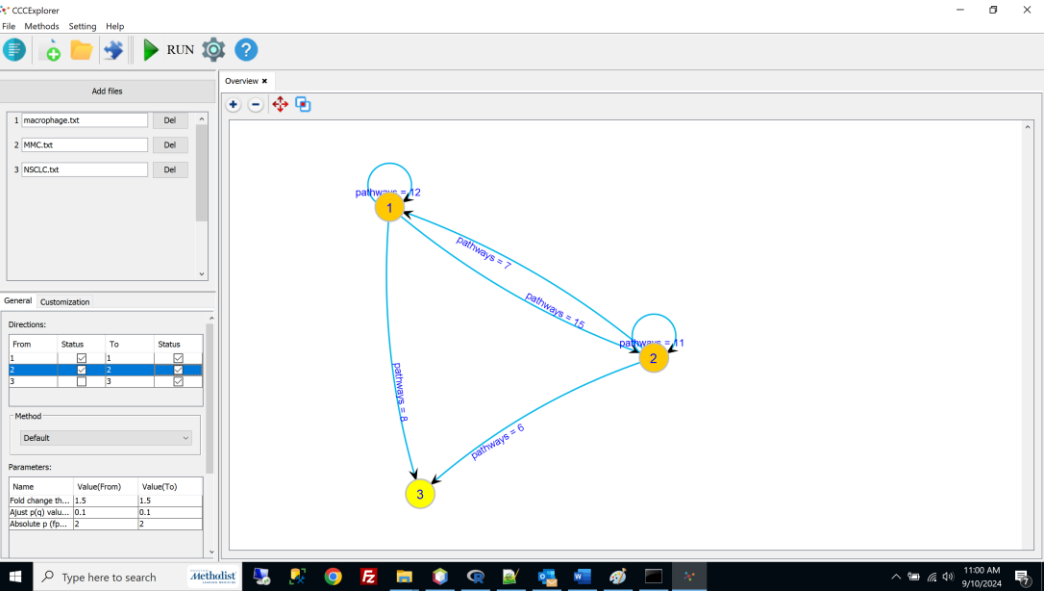
Figure 5

User can check the common pathways and common ligand-receptor pairs by clicking the icon in the Figure 6.
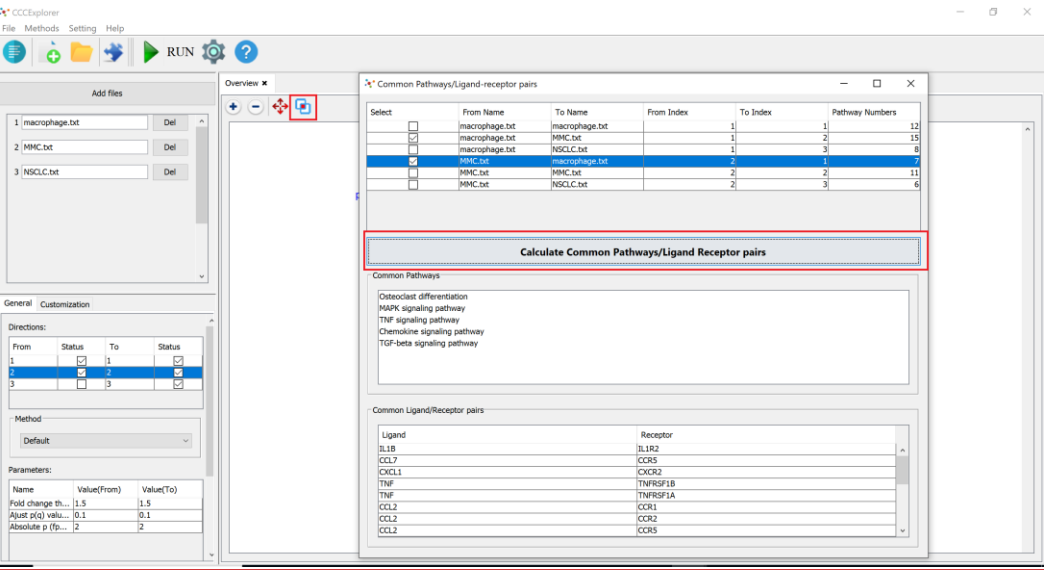
Figure 6

When user click the pathway of the Figure 5, user can see the output details of the selected direction, eg. Figure 7.

The red box 1 in the Figure 5 is the pathway network. will display in the red box 1 on Figure 5.

TheIn the red box 2 , it is p value information of pathway.

TheIn the red box 3, it is the mapping of ligand and receptor.

The red box 4 is the toolbar of output window. User can zoom in, zoom out, invisible pathway and export the pathway.

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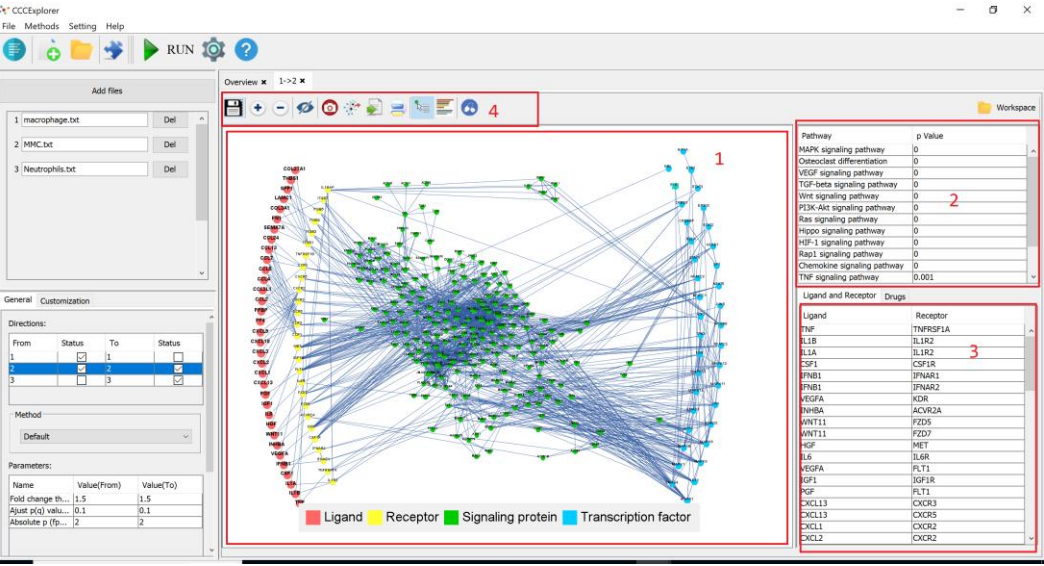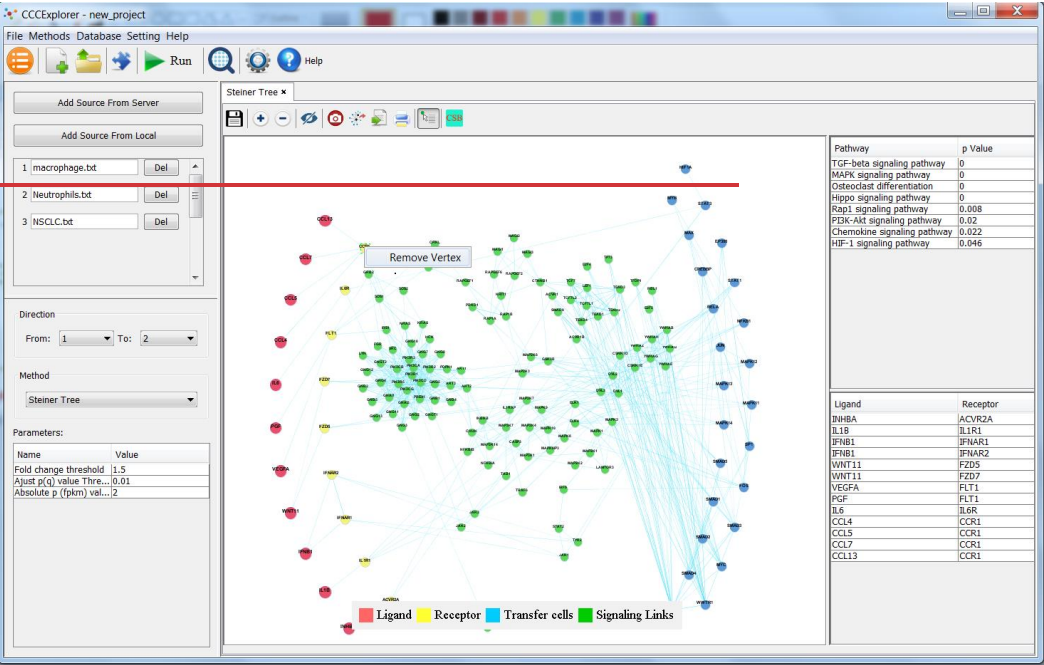Draft by Xiaohui Yu 09/1006/202416
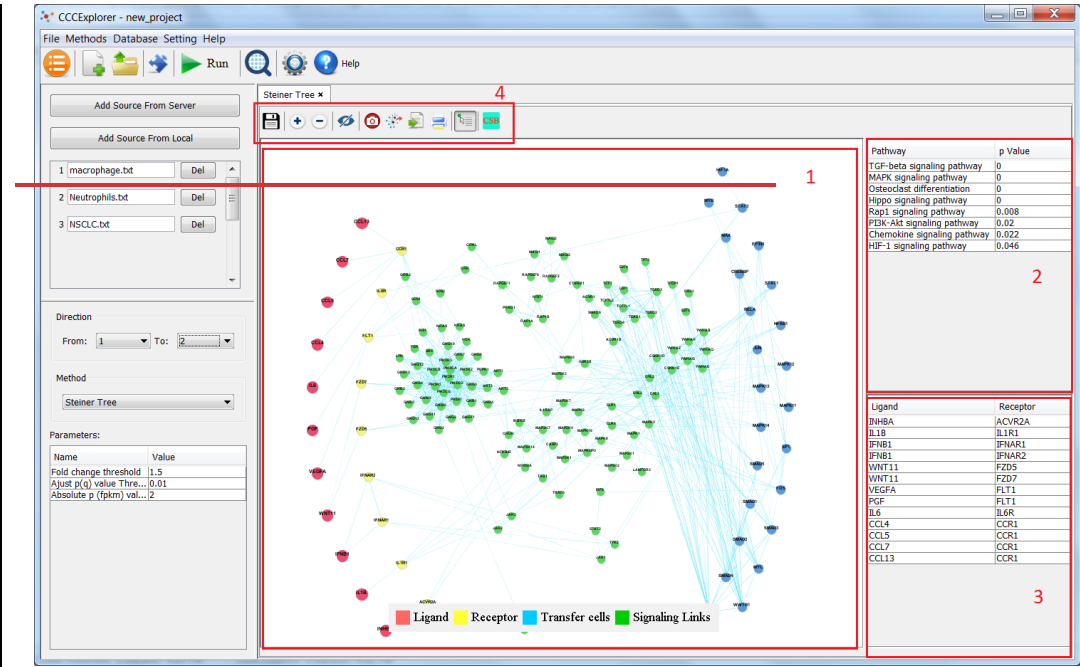
Figure 57

User can right click on a gene node on the pathway network to delete a gene node to see the changes of pathway network. Eg. Figure 86.
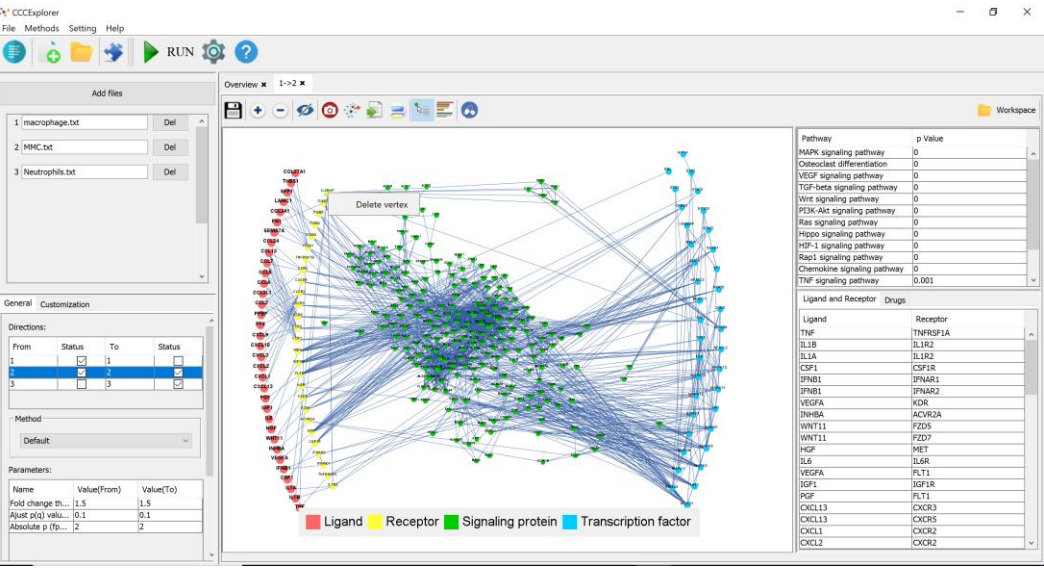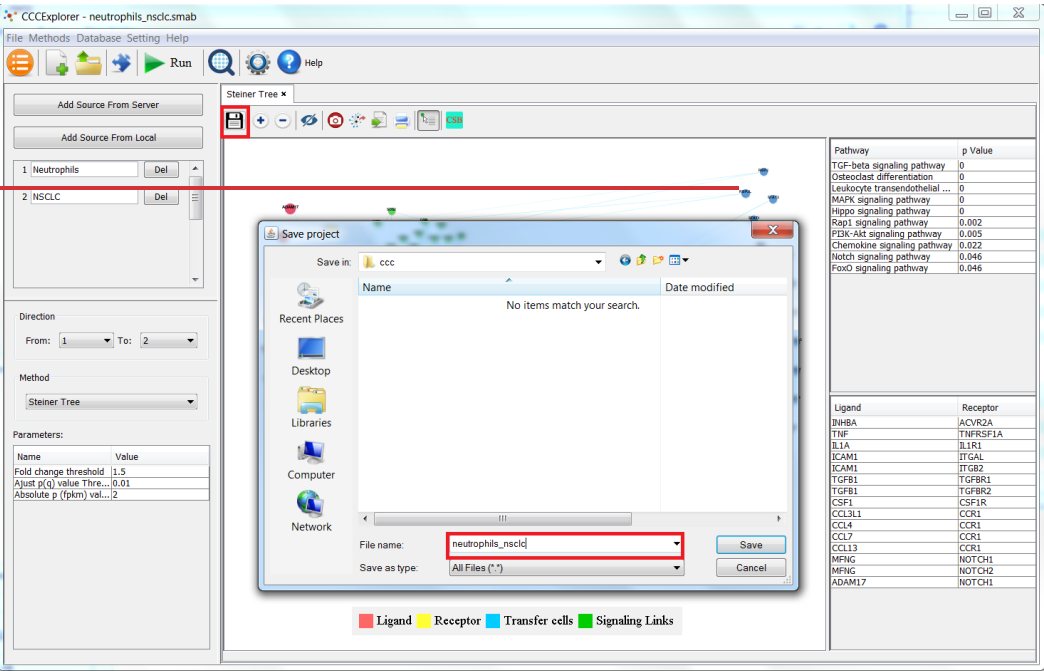
Figure 8~~6~~

Save a project

To save a project, user can click on the save icon on the toolbar of output window. And then give a project name. Eg. Figure 9~~7~~.
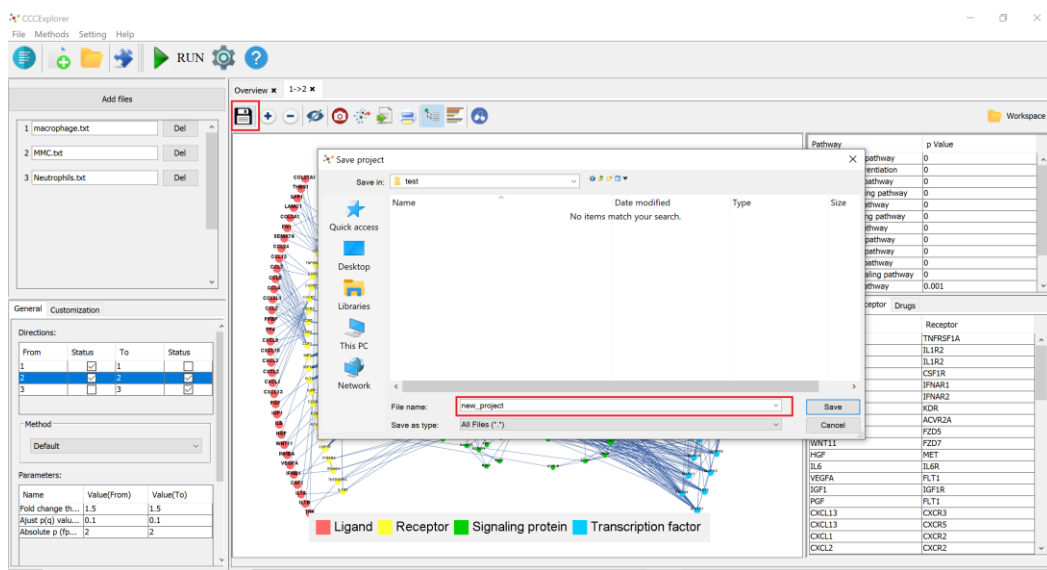
Figure 9~7~

There are several files will be created after clicking save button. The file list is in Figure 10~8~. The .smab file is the project file. User can open this file with CCCExplorer to load a project.
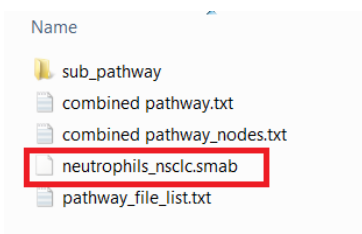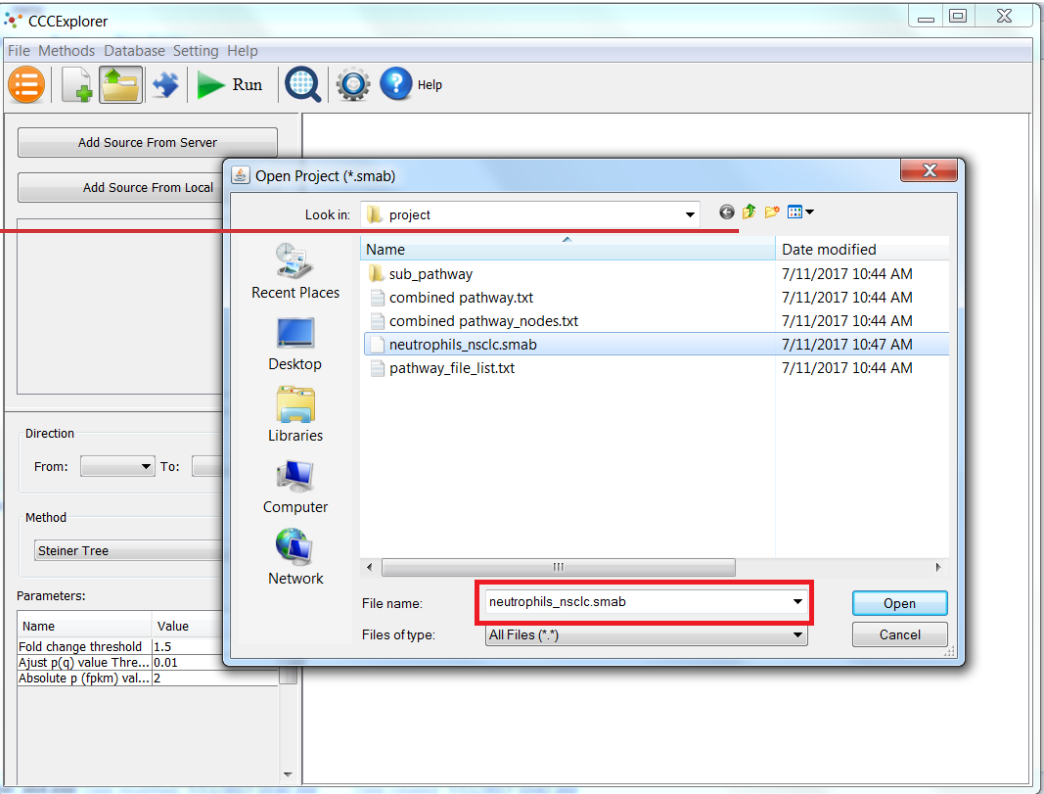

Figure 10~8~

Open an existing project

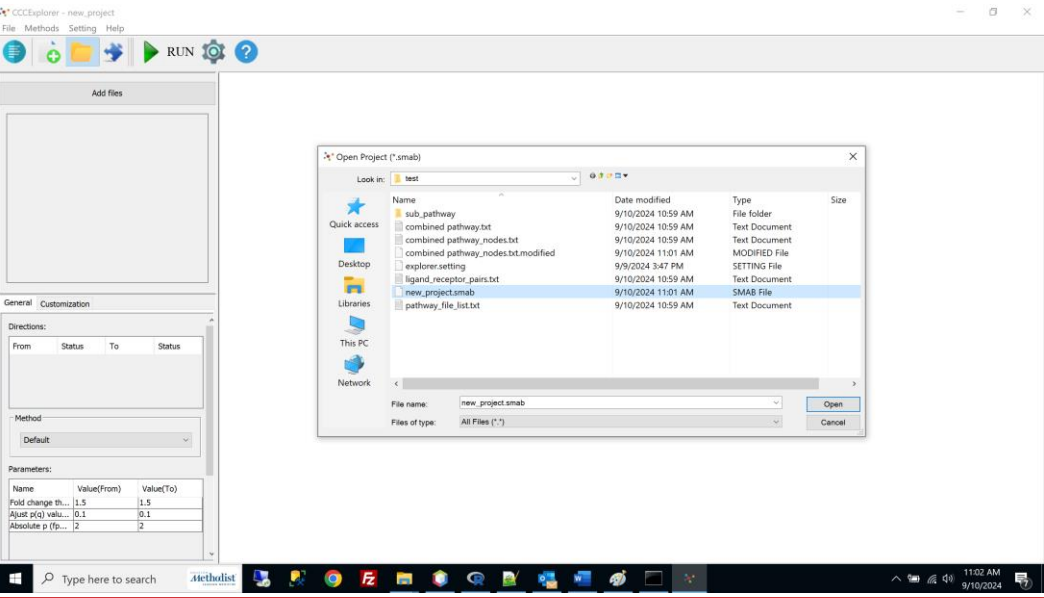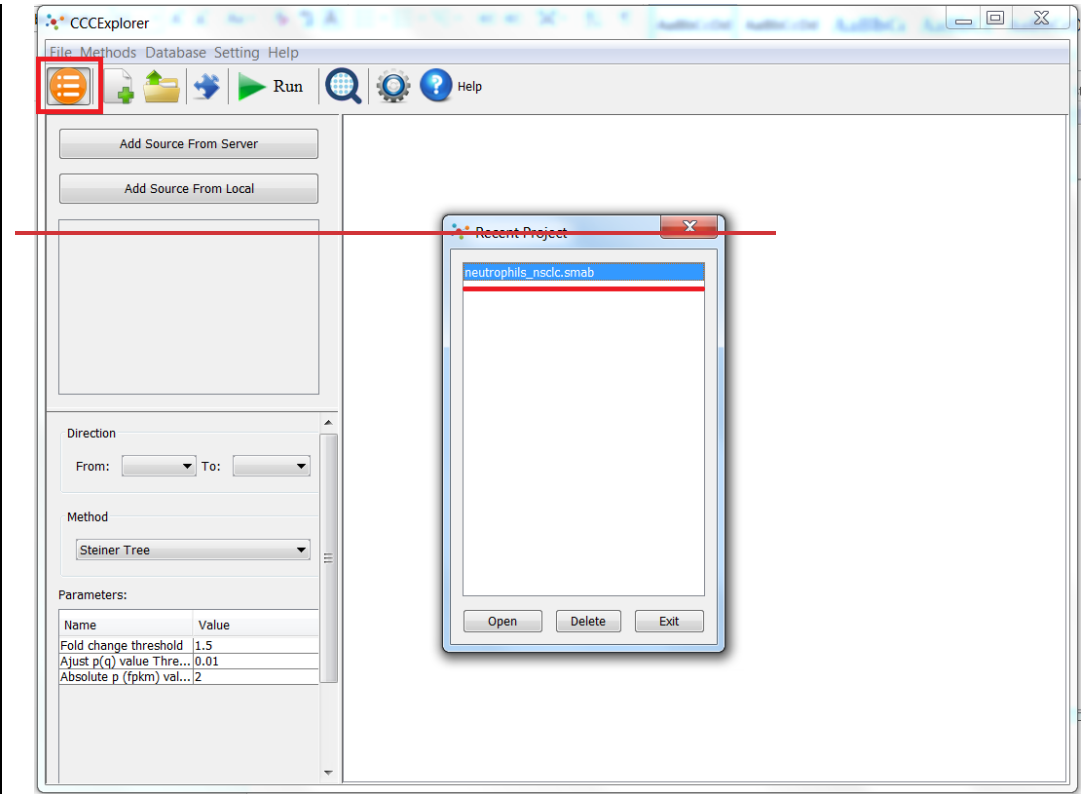Clicks on the folder icon on the toolbar of main window and select a project file as figure 11~9~.

Figure 119

User also can open a project from the recent project list. Click on the first icon on the toolbar of main window to open it.
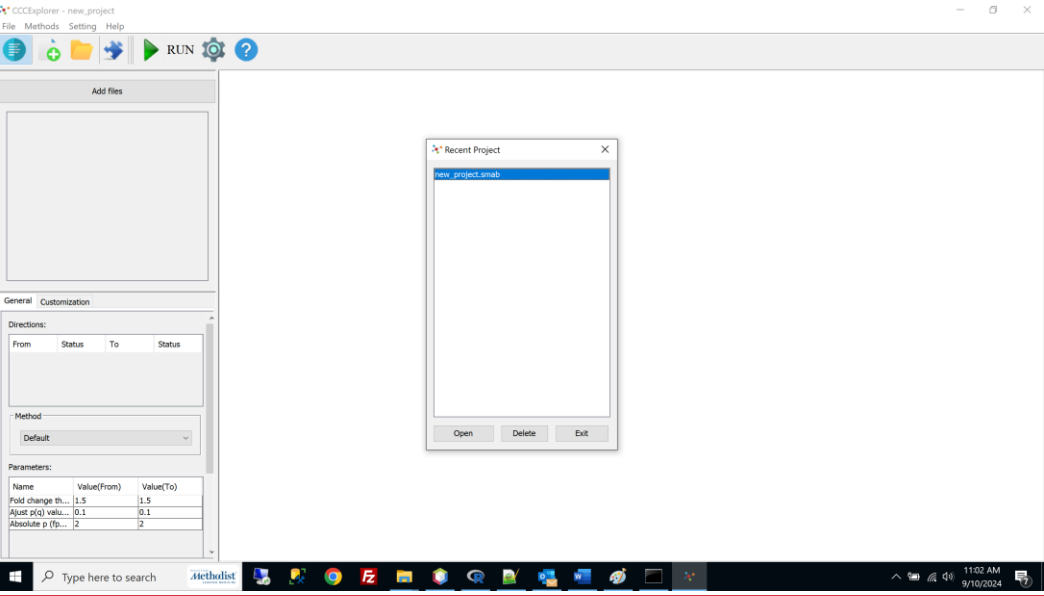
Figure 120

Add a method

To add a new method into CCCExplorer, user needs to provide two files. One is the configuration file, the other is algorithm program. Currently we support the R language based algorithm program. The configuration file is JSON format. User can create a method configuration file according to the interface format of the algorithm file.

The figure 131 is the structure of the configuration file.

```
   CCCExplorer_steiner_tree.R   steiner_tree.conf

        0         10        20        30        40        5
 1  {
 2  "algorithmName":"Steiner Tree",
 3  "fileName":"CCCExplorer steiner tree.R",
 4  "entryFunctionName":"CCCExplorer",
 5  "paramsArray":[
 6  {
 7  "description":"Fold change threshold",
 8  "defaultValue":"1.5"},
 9
10  {
11  "description":"Ajust p(q) value Threshold",
12  "defaultValue":"0.05"},
13
14  {
15  "description":"Absolute) value Threshold",
16  "defaultValue":"2"}
17  ]
18  }
```

Figure 131

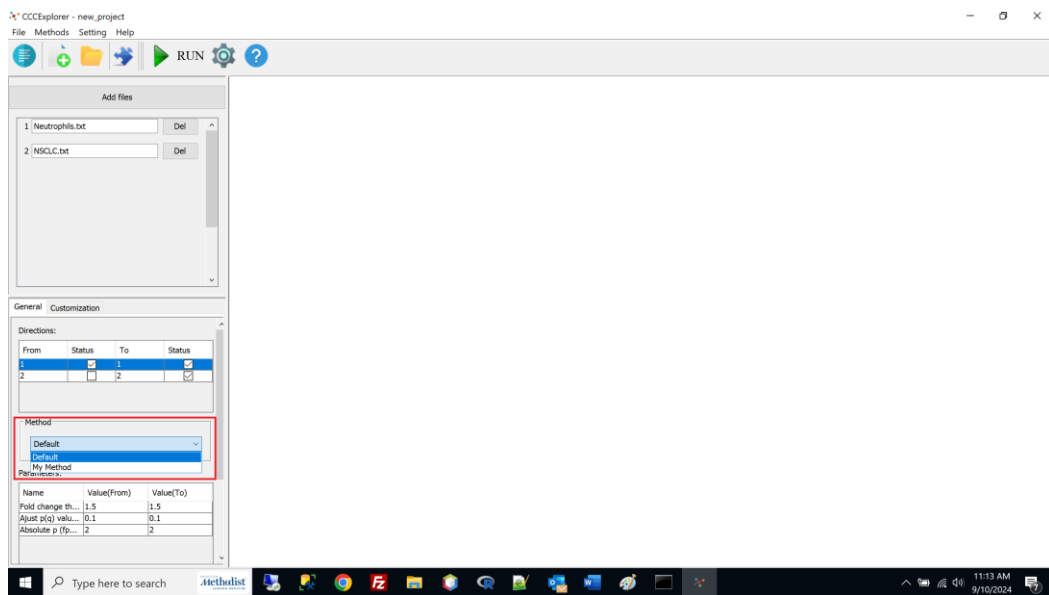Figure 142 is the mapping relation between the configuration file and the display UI.

Figure 1~~2~~
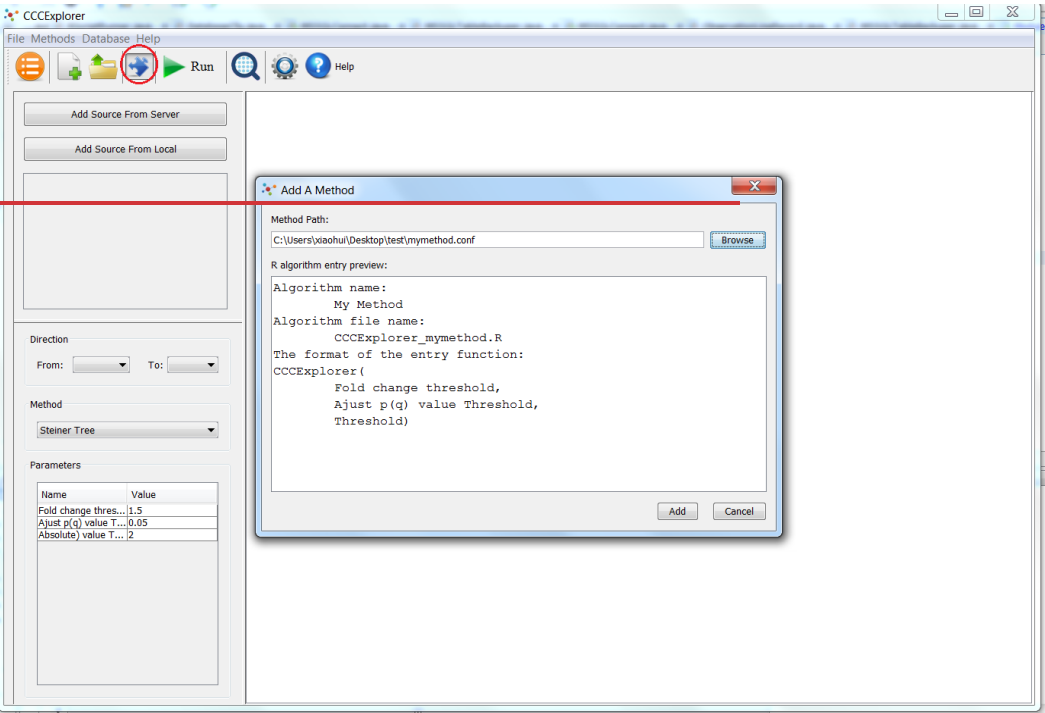
Click on "Methods->Add Method" to select a method configuration file~~,~~ eg. Figure 15.~~-~~ User needs to make sure the algorithm program is in the same folder as the configuration file.

From the preview box, user can check whether the format of the method is correct.
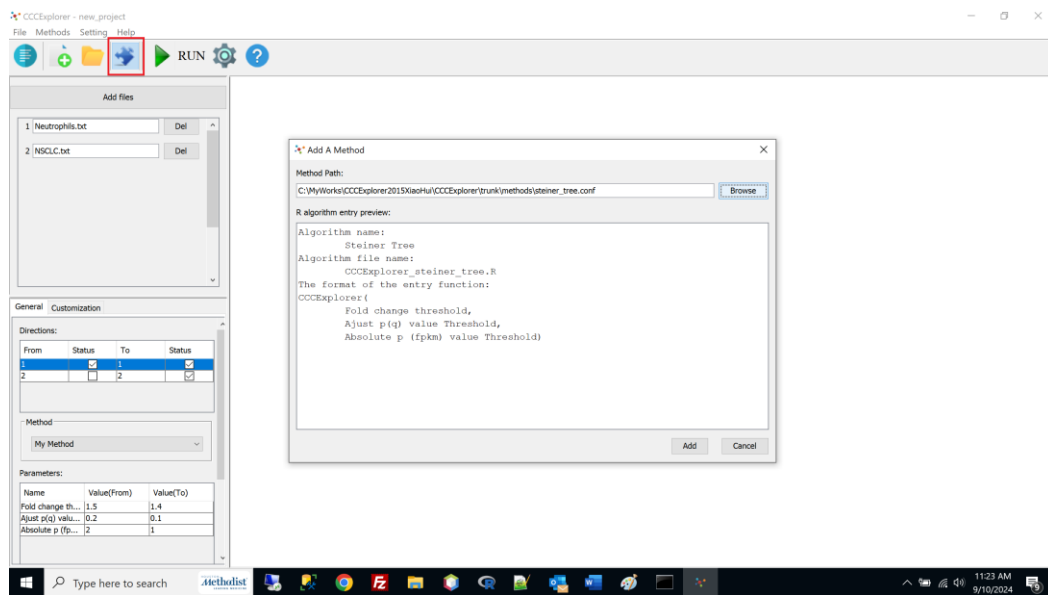
Figure 13

After adding a new method, user can choose the new method from the left-side panel like the figure below.

Figure 1~~5~~4

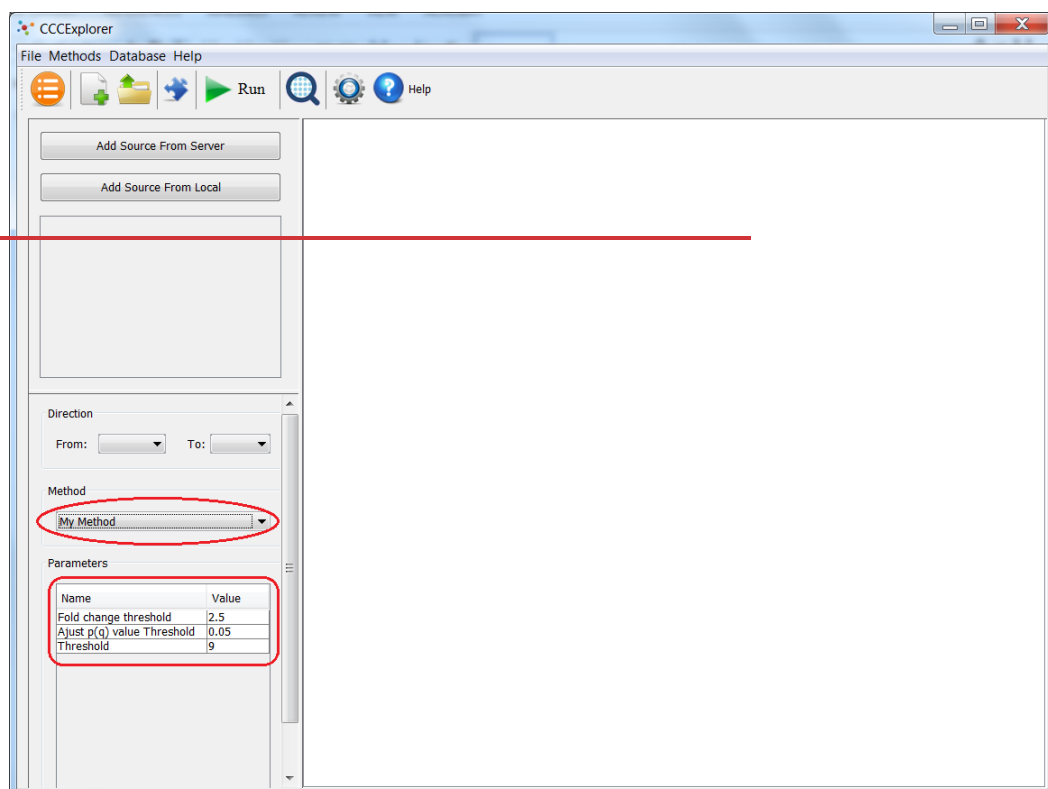## The format of the output files

There are three files and one folder that the algorithm program needs to generate.

Figure 1~~6~~5

The file "combined pathway.txt" contain the pathway information. The figure below is the format of this file.

```
combined pathway.txt
     0         10        20        30        40
  1 From   To   Direction Interaction_type
  2 TNF TNFRSF1A  directed  LR
  3 IL1A   IL1R1 directed  LR
  4 IL1R1 IL1RAP  directed  heterodimer
  5 CHP1   NFATC1  directed  process(activation)
```

There are 5 columns in this file. The delimiter of each field is tab character \t.

The file "combined pathway_nodes.txt" contain the node information. The figure below is the format of this file.


```
combined pathway_nodes.txt
    0         10        20        30        40        50        60        70        80        90
  1 gene   gene_type pathway
  2 NFKBIA   links Osteoclast differentiation;TNF signaling pathway;NF-kappa B signaling pathway
  3 PLCG2 links Osteoclast differentiation
  4 PPP3CA   links Osteoclast differentiation
  5 PPP3CB   links Osteoclast differentiation
  6 PPP3CC   links Osteoclast differentiation
  7 PPP3R1   links Osteoclast differentiation
```

There are 3 columns in this file. The delimiter of each field is tab character \t.

The file "pathway_file_list.txt" contain the sub pathway information. The figure below is the format of this file.


```
pathway_file_list.txt
    0         10        20        30        40        50        60        70        80        90        100
  1 Osteoclast differentiation   0.007 Osteoclast differentiation_nodes.txt   Osteoclast differentiation.txt
  2 TNF signaling pathway 0.014 TNF signaling pathway_nodes.txt TNF signaling pathway.txt
  3 NF-kappa B signaling pathway  0.019 NF-kappa B signaling pathway_nodes.txt  NF-kappa B signaling pathway.txt
  4 MAPK signaling pathway  0.048 MAPK signaling pathway_nodes.txt  MAPK signaling pathway.txt
```

There are 4 columns in this file. The delimiter of each field is tab character \t.

The first column is the name of sub pathway.

The second column is p value.

The third column is the file name of node for sub pathway. It contains the node information of sub pathway.
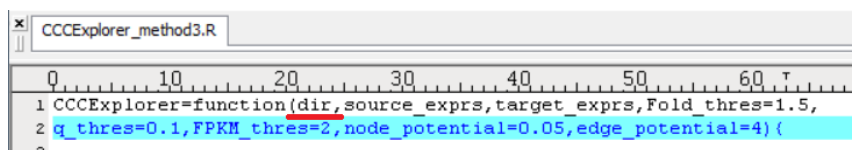
The forth column is the pathway file name of sub pathway. It contains the pathway information of sub pathway.

Algorithm program needs to create a folder named "sub_pathway" and put all the node and pathway information of sub pathway into it.
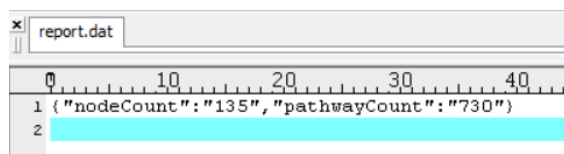
Note that:

1. The first parameter of the algorithm program is the path in which all the output files will be put.

The figure below is the example of an R algorithm program.

2. The algorithm program also needs to create a report file (report.dat) in the current workspace before it returns. The format of the report file is JSON forma.

Drug Discovery

When user clicks drug toggle button, the genes on which has drugs target will be highlighted, eg. Figure 17. User can move the cursor on the drug to see the drug information. When the user moves the cursor between the genes, the drug list will be updated.

To lock the drug list, user needs to double click a drug, then user can double click any drug in the drug list, the CCCExplorer will open the drug-bank website to show the details of this drug.

To unlock the drug list, user only needs to single click any gene.

~~Delete a method~~

~~Go to "Methods->Manage Methods" to delete a method. User can only delete the own method. Cannot delete a system method.~~
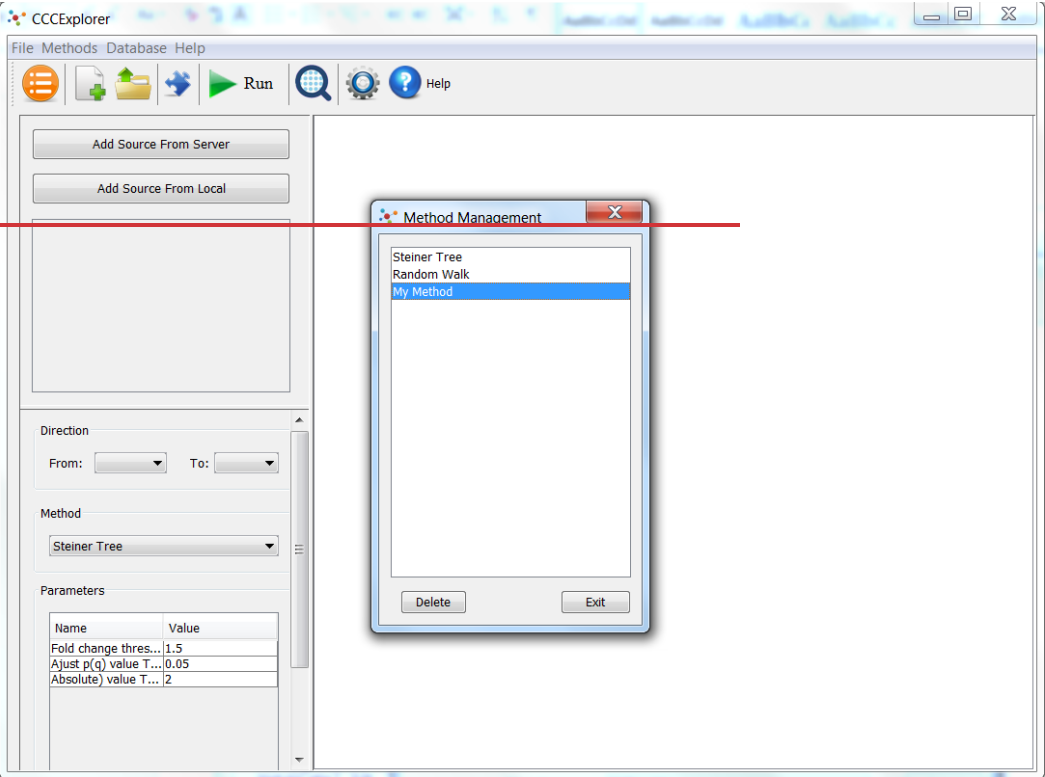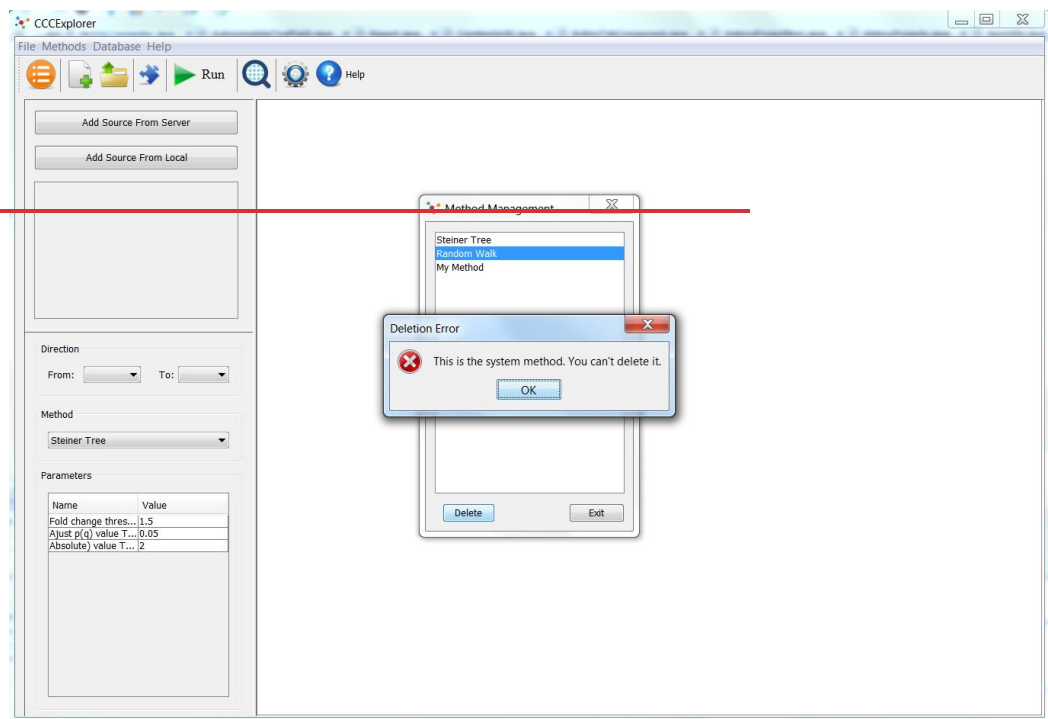
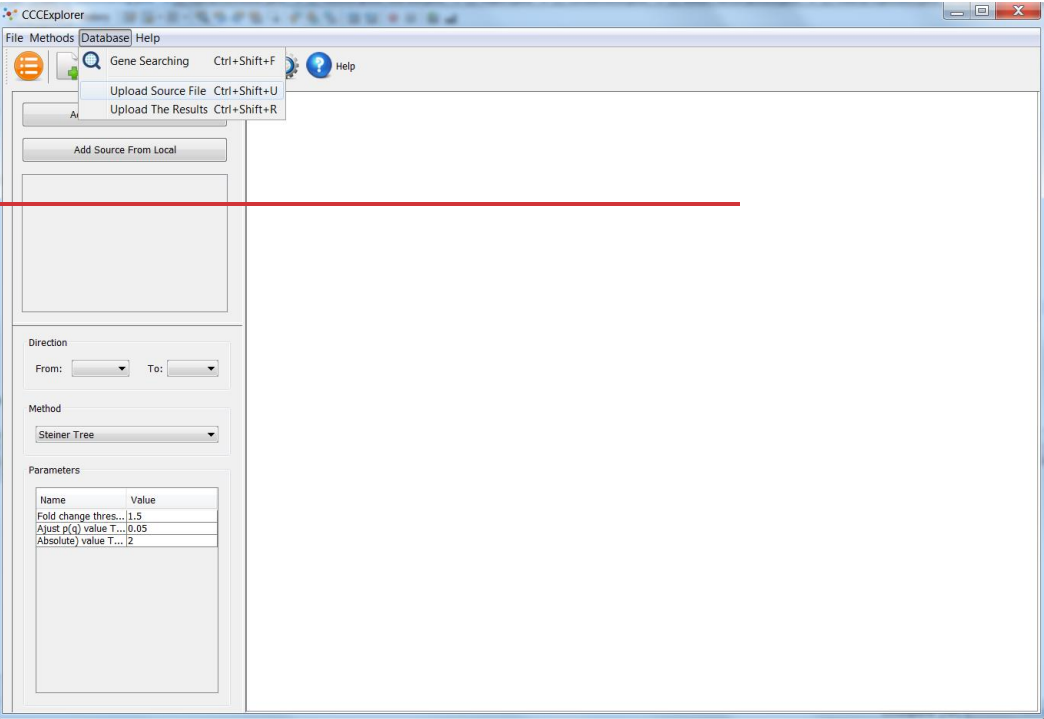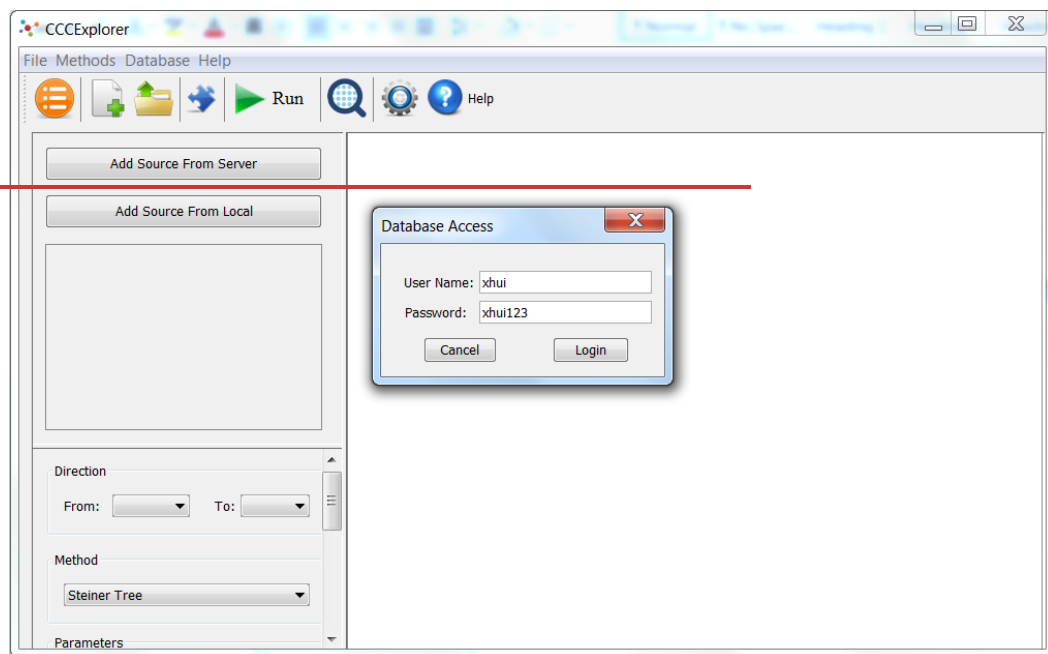## Upload a data source

This feature is for an administrator.

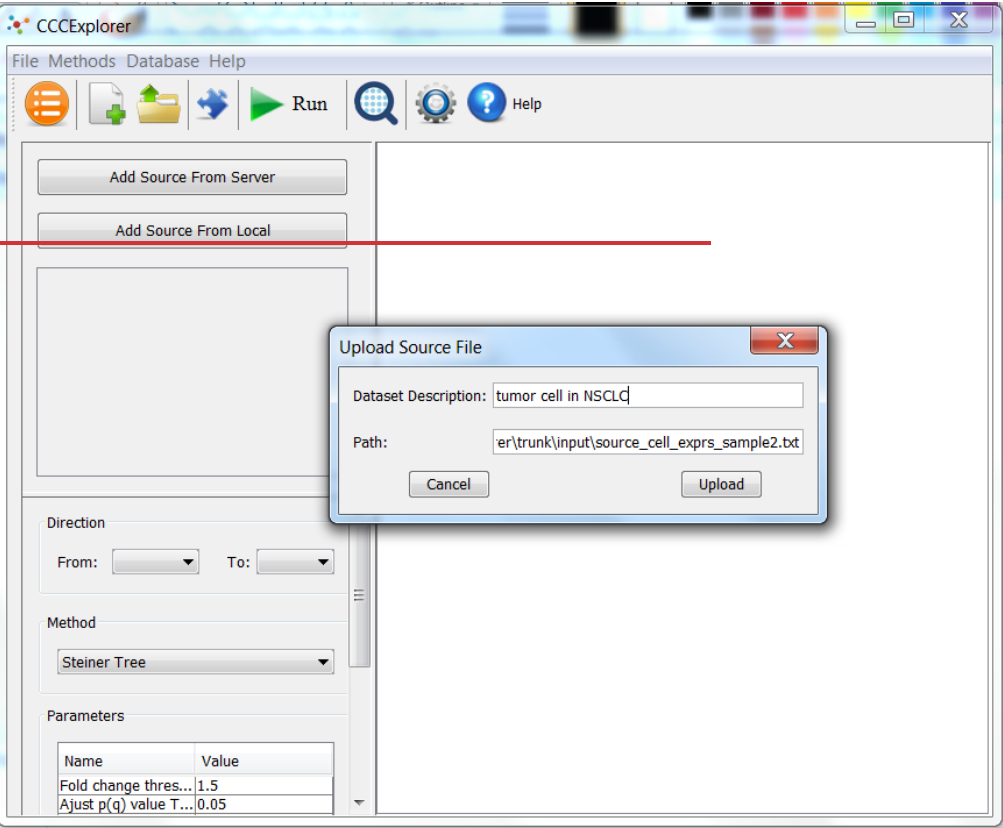An administrator can upload the data source and the result to the remote database.

Go to "Database->Upload Source File" to select a data file. CCCExplorer will verify the user before uploading the file.

User needs the user name and password to access the remote database.
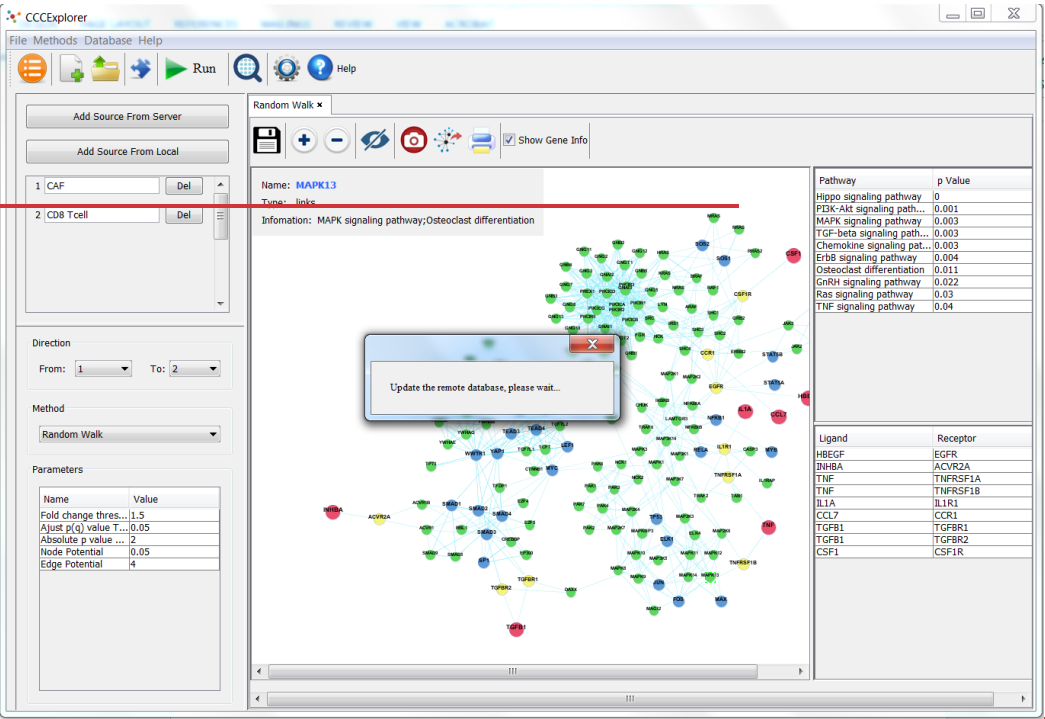
~~User needs to give a description for the dataset.~~

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Figure 17