InterMineR Cytoscape Interface

InterMine University of Cambridge

Celia Sánchez Laorden csanchla8@alumnes.ub.edu

Source: InterMineR Cytoscape Interface is on Github

December, 2020

This interface wants to be a guide to run queries and interpret them with the intuitive Cytoscape visualizations without prior software experience. It facilitates understanding and communication of relevant relationships between different biological Data Classes.

Contents

1	Req	quirements							
2	Cap	pabilities							
3	Basic Usage								
	3.1	Overview							
	3.2	1.1 Templates tab							
	3.3	1.2 Query Builder tab							
	3.4	2. Run your query tab							
	3.5	3. Visualize your results tab							
	3.6	4. Overlay additional data tab							
	3.7	Saved Networks tab							
4	Sou	arce Code							

1 Requirements

InterMineR Cytoscape is an interface created with Shiny. All code is available from: Github. To run the Shiny app, first, make sure that you have installed:

- 1. R Studio version 4.0.3 or above.
- 2. All the files and the "www" folder from the GitHub repository. Unzip the folder. Set your working directory to the unzipped folder once in R Studio (see setwd function).
- 3. All of the packages from the Packages.R file in R Studio. In order to install them correctly, run the installation for each package in turn.

Open R Studio, open the file app.R and open the file $workspace_app.RData$. Then, press "RunApp".

2 Capabilities

Using this app you will be able to:

- 1. Run queries using any template from all registered InterMine instances in one place.
- 2. Advanced users can use a flexible query interface to construct their own data mining queries.
- 3. Display and export the results in a table.
- 4. A set of network visualization tools from Cytoscape domains enrich the interpretation of the results.
- 5. Further options allow customization of the Cytoscape Networks.
- 6. Store your visualizations in JSON format and display saved Networks.

3 Basic Usage

The InterMineR Cytoscape Interface divides the tasks into seven tabs:

- **Home**: contains a short walk-trough the app.
- Create your query: here you can select either Templates, which allows you to select predefined queries. Or Query Builder, which provides a tool to flexibly create your own queries.
- Run your query: displays the results from the query previously created.
- Visualize your results: is a Cytoscape Network viewer.
- Overlay additional data: is the tool to style the Network chart.
- Saved Networks: enables you to visualize the results you have saved from past queries.

3.1 Overview

On the left side of the screen there is a sidebar menu, where in addition to the tab menu, a select list enables you to choose a registered InterMine instance. In the upper right corner, there is an information button that takes you to the source project in GitHub and redirects you to a place where you can expose any issue you find.

In each tab panel, you will find a help button. When you click to the question mark? icon step-by-step instructions will be displayed. Some hints are also visible by hovering your mouse over the buttons.

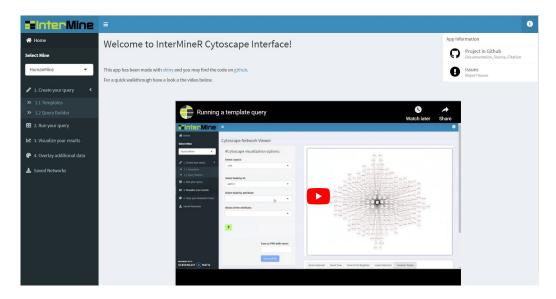


Figure 1: InterMineR Cytoscape Interface Home tab.

Each tab will be explained in more detail below:

3.2 1.1 Templates tab

You first will need to select a query from the list of templates. At this point, you will see the predefined constraints of the template in the main panel of the tab. You can change the value by default and this way modify the constraints.



Figure 2: Pre-defined constraint for the Template Protein-->Interactions from HumanMine.

A summary table of the constraints selected is displayed. Each time you select a new template query, all the modifications are deleted, and you can start again. To go to the next section, click **Go to Results** at the lower right corner.

3.3 1.2 Query Builder tab

The Query Builder modality is only encouraged for experienced users. To start building a query from scratch, first, you will need to define a Data Class. Then, you must set which attributes you want to see in the results. This also defines the type of sorting which will be used to order the retrieved data frame. At the bottom of the page, you can change the predefined choice of ordering and select if you want to sort the results in ascending or descending order. Setting a constraint for the first Data Class is optional, but take into account that at some point you will need to define one. At this point, if you are defining a constraint you can type multiple values separated by commas. Just a clarification: the constraint operator and value(s) that you enter in the boxes below your first Data Class choice run against this class. If you press the Constraints button you can set a constraint against an attribute from the first Data Class. You can only select one attribute, otherwise you will get an error.

Press the Set button if you want to add a second level, dependent on your first Data Class choice, and overlay extra data. In the consecutive steps, one checkbox tree is displayed for the data type to be returned and another one for data types to set constraints. In the first tree, Type of data to be returned, you can select the data you want to see in the results table. If you want to set a third level, pressing the Set button below the trees,

you could need to select the data types in the second level that you do not want to see displayed in the results table. Do not worry, you can delete these data types after setting the third and consecutive levels pressing Set Query button. When you press this button, a emergent window will appear with all the values that are going to be seen in the results table. By selecting the ones you want to remove and pressing Delete Rows button you will get rid off any undesired data type.

Once you have achieved the 3rd level, you can press the Overlay extra data button to set two more levels of extra data into your query. Pressing Set Query button, apart from removing selected values, will show you a summary table with the constraints you have defined. If you have built a query that can be run against the InterMine instance you will be able to press in the lower right corner the Go to Results button that will take you to the next section.

3.4 2. Run your query tab

In this section, a table containing the data which were retrieved from the InterMine instance is displayed. You will need to select the Set Nodes and Edges button to select the Id and the Source for the Cytoscape Network Visualization. The Id and Source need to be different. At this point, you may also want to define the Node Attributes to then be able to manipulate the network chart according to filtering criteria given by these attributes.

3.5 3. Visualize your results tab

Here, you can set different visualization and filter options. First, you can choose different layouts from the Select Layout list. Specific nodes from your network can be selected by attribute or ID, using buttons at the left of the page. Buttons below the network allow various actions based on the nodes selected: Remove Selected (you can go back and display all the initial nodes pressing the Show All button), zoom selected, reset the view or select the first neighbour of a node or a selection of nodes. In addition you can invert the selection, unselect nodes and display a list of names from the selected nodes.

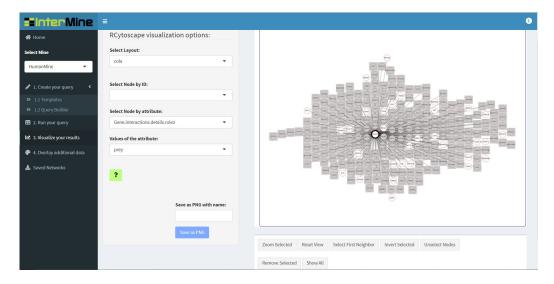


Figure 3: Caption of the Visualize your results tab.

3.6 4. Overlay additional data tab

In this last tab, you can easily style the network chart. In the Node's body menu first, select which parameter you want to customize using Set Parameter. Second, you need to define the value for the parameter. You can either set the node(s) to customize by their ID or by an attribute. You can select one of the attributes set in the Run Query Section to filter the customization. You must select the Value for the attribute if you have chosen this way. Each time you describe a new feature for the network do not forget to press the Customize the Network! button. Pressing History of changes button you can see the changes you have made and delete some of them by pressing Delete Rows.

Finally, you can save your results as a static image, in PNG format, using the Save as PNG option. Saved Networks can be uploaded in the Saved Networks tab. If no name is provided for the image a default name will be given. In addition a ZIP folder with the files for an interactive network display can be saved using the Save as ZIP option in the Style your network charts tab. Again, if no name is provided a default name will be given. The ZIP folder will contain the results of the query in a CSV file, two CSV files with the basic components and the modifications made to the Network and a JSON file of the Network.

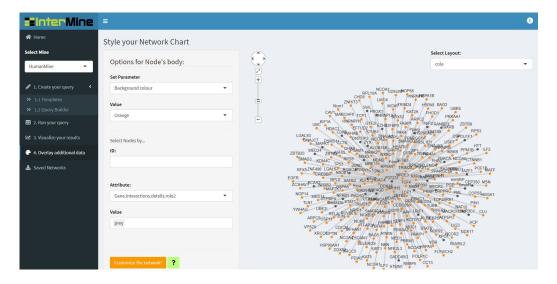


Figure 4: Caption of the Overlay additional data tab. The background colour of the nodes corresponding to genes that in the interaction have a prey role that is set to orange.

3.7 Saved Networks tab

In this last tab, you can display previously saved networks. You will need to press Browse... and navigate to find the zip folder you have saved in the tab Overlay additional data. Then, you will need to press Unzip files and the results of the query in a table and the network chart will be displayed.

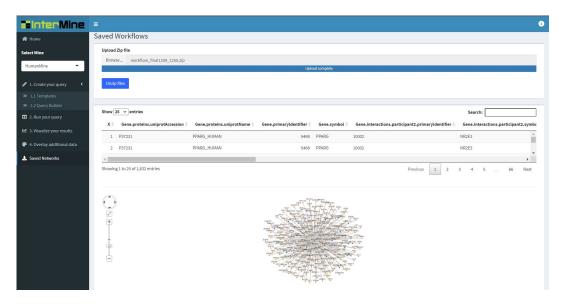


Figure 5: Caption of the Saved Networks tab displaying the example Network chart shown in Figure 4.

4 Source Code

InterMineR Cytoscape Interface is open source and may be downloaded and forked on Github. Pull Requests are welcome!