

PathBubbles

Version 1.0

Manual

Yongnan Zhu

E-mail: yongnan@umbc.edu

November 16, 2014

Introduction

PathBubbles is a web-based application of biological pathway visualization and analysis, allowing users to visualize, search pathways from Reactome, to upload their own gene data for ortholog analysis, and to upload their gene expression data for expression analysis. This is a web-version of PathBubbles project: <https://sites.google.com/a/umbc.edu/pathbubbles/>.

The current version is "1.0".

It is freely available at <http://raven.anr.udel.edu/~sunliang/PathBubbles/> (see Figure 1).

All the code is hosted on Github, you can fork it through the link: <https://github.com/yongnanzhu/PathBubbles>.

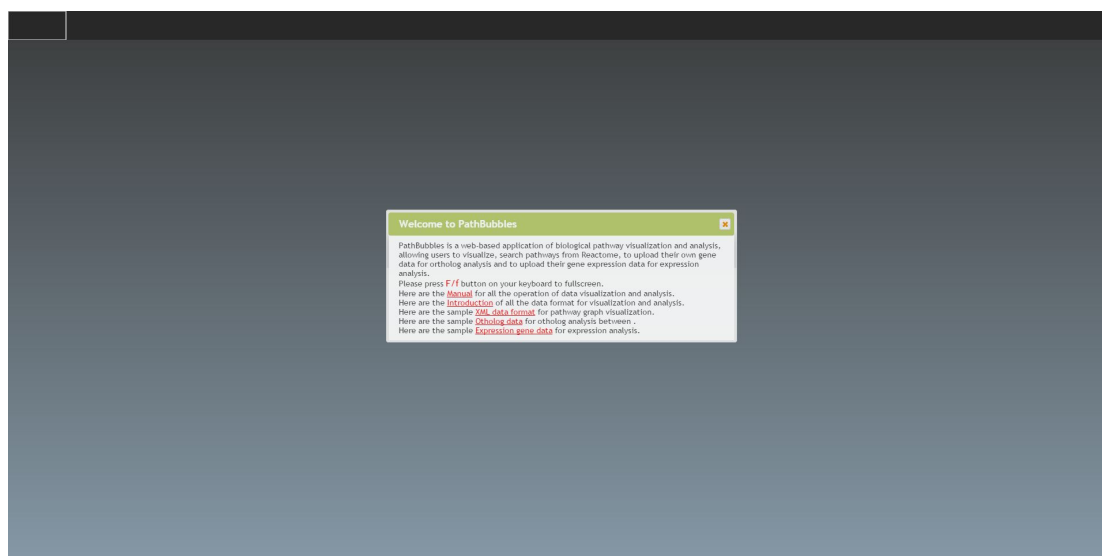


Figure 1 homepage of PathBubbles

Browser requirements

All modern ones, such as Safari, google chrome (best), and IE are supported. Please do not use FireFox. You can visit [Google support](#) for more information.

Supporting Pathway network format

The pathway graph in Pathbubbles supports pre-defined XML format.

We will first show you the sample example, and then tell you the detail format.

```
<?xml version="1.0" encoding="utf-8"?>
<Pathway>
```

```

    <compartmentBlock Num="3">
      <compartment j="0">
        <Name>early endosome membrane</Name>
        <Position>(0.40767891088437735,0.2510594446429637,0.18464217823124535,0.2294125895309596
4)</Position>
        <Contain>(C,1,,S,1,,S,14,,S,4,,S,6,,S,8,,S,9,,S,15,,S,16,,S,19,,S,20,,S,24,,S,26,,S,29,,S,30,,S,34,,
S,36,,R,1,,R,2,,R,3,,R,4,,R,5,,R,6,,R,7,,)</Contain>
      </compartment>
    </compartmentBlock>
    <complexBlock Num="7">
      <complex j="1">
        <Name>PIKFYVEVAC14FIG4</Name>
        <Position>(0.6283649298613249,0.5706117201901926,0.042311567567274076,0.027386127875
258303)</Position>
      </complex>
    </complexBlock>
    <physicalEntityBlock Num="1"/>
    <proteinBlock Num="15" />
    <DnaBlock Num="1"/>
    <RnaBlock Num="1"/>
    <smallMoleculeBlock Num="37"/>
    <reactionBlock Num="9">
      <reaction j="1">
        <Name>PI(34)P2 is dephosphorylated to PI3P by INPP4AB at the early endosome
membrane</Name>
        <Type>T</Type>

        <Position>(0.41048415733565263,0.2221266133316178,0.016924627026909632,0.0273861278
75258303)</Position>
      </reaction>
    </reactionBlock >
    <edgeBlock Num="41">
      <edge j="0">
        <Name>A</Name>
        <Ends>(P, 1, R, 1)</Ends>
      </edge>
      <edge j="39">
        <Name>J</Name>
        <Ends>(R, 8, S, 36)</Ends>
      </edge>
    </edgeBlock>
  </Pathway>

```

The first line is about the standard xml tag. The formal pathway is a hierarchical structure.

The first type is compartment. Compartment has attributes with “Name” ,” Position” ,” Contain” . The position is a string with the combine of “x” , “y” , “w” , “h” of this compartment. For the “Contain” ,it is consisted of all the biomolecules of the compartment. Which is splited by “;” . For each biomolecule, it begins with its type, and id. The id is the index of this type.

In PathBubble, it has 6 types.

“C” for complex;
 “P” for protein;
 “D” for Dna;
 “Rna” for Rna;
 “E” for “PhysicalEntity” ;
 “S” for small molecule;
 “R” for reaction

For each biomolecule, it has its id for “j” attribute.
 Its “Name” , its “Type”

At the end of the file is about the edges, which tells you the “Name” of the edge and Its two endpoints.

The endpoints is begins with the type of Biomolecule and the id of biomolecule, and ends with the type of Biomolecule and the id of biomolecule.

Supporting Pathway ortholog gene data format

You can upload you own gene data for ortholog analysis in PathBubbles.
 Below we will you show the gene data format, which is tab-delimited format. The first column is about the symbol of gene, and the second column is about the database Id of this gene.

```

symbol dbId
ADA      \N
CDH2     414745
AKT3     421497
MED6     426282
NR2E3    395289
  
```

Supporting Pathway gene expression data format

You can upload you own gene expression data for expression analysis in PathBubbles.

Below we will you show the gene data format, which is tab-delimited format. The first column is about the gene id, the second column is about the symbol of gene, and the third column is about the log based ratio of this gene in expression experiment.

gene_id	symbol	ratio
374096	SMAD6	0.6892992938620315
395132	SMAD3	7.128911138923654
395247	SMAD2	3.370212765957447
395543	SMAD9	Infinity
395679	SMAD5	3.013579576317219
395680	SMAD4	2.3619197482297403
429683	SMAD7	0.647887323943662
374094	TGFBR1	6.733865119651922
396399	TGFBR2	0.45263157894736844
395934	SHC1	1.4310163243812535
426482	SHC4	Infinity
431265	SHC3	NaN
770341	SHC2	3.3697916666666665
386572	GRB2	10.56062819576333
423572	SOS2	1.4514200298953663
425964	SOS1	1.5194805194805194

Introduction of PathBubbles interface

1. Full screen

You can press “F/f” on your keyboard to change to “full screen” Mode. If it is on the “full screen” Mode, you can press “Esc” on your keyboard to exit the “full screen” Mode.

2. Menu of the scene

In PathBubbles, If you right click on the scene, it will pop out a menu. (see Figure 2).

You can view pathway network graph by select “Open bubble” menu, You can view all the pathways in a tree-ring by select “Open treeRing” menu, you can open help menu by select “Open help menu” and you can delete all the bubble on the scene.

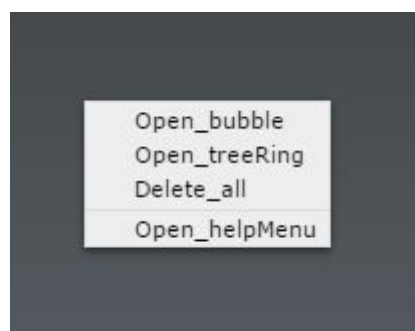


Figure 2

3. Menu of the Bubble

In PathBubble, all the bubble can be group and ungrouped, and also can be deleted. For certain Bubble, you can click “M” to open its function menu.

(1) Open Tree Ring

You can view all the pathways in a tree-ring by select “Open treeRing” menu.

It will show you the default view. (see Figure 3)

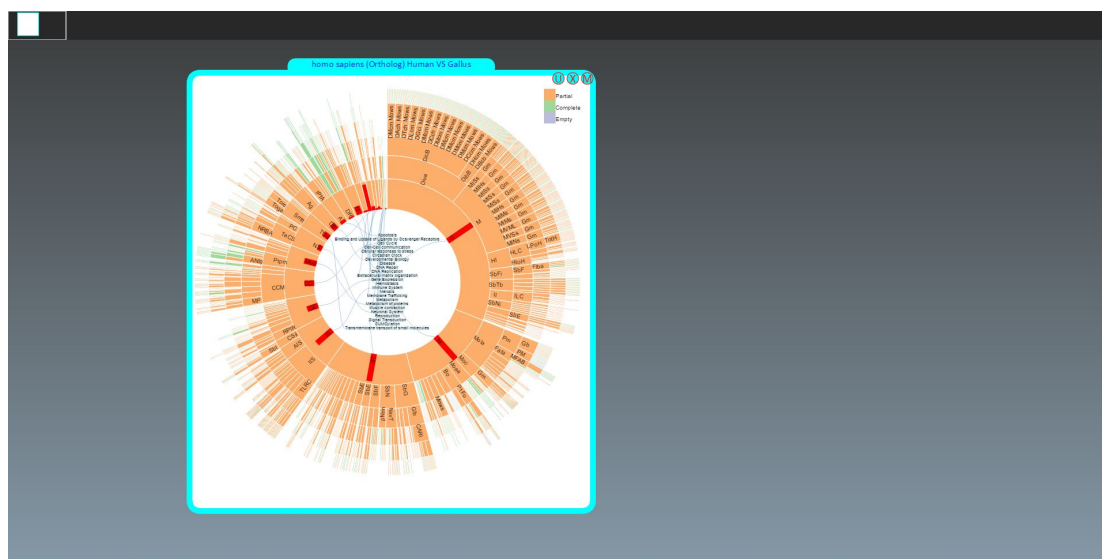


Figure 3