

Multiomics Data Mapper (Input files)



This gadget merges Shimadzu multi-omics data with gml file of blank molecular pathway. The integrated gml file is used as input to VANTED gadget to visualize the multi-omics data on the molecular pathway map.

(1) Pathway GML File
transomics_plane_map_withID0125.gml

(2) Shimadzu Multi-omics Data
test_multi_omics_a.szf

compound name	ChEBI	Inchi	KEGG_COM
(Sample No)	*	*	*
G6P	CHEBI:4170	NBSCHQHZLSJFNQ-GASJEMHNSA-N	C00092
R5P	CHEBI:52742	KTVPXOYAKDPRHY-SOOFDHNKSA-N	C00117
E4P	CHEBI:48153	NGHMDNPXVRFPGS-IUYQGCFVSA-N	C00279
S7P	CHEBI:15721	JDTUMPKOJBQPKX-GBNDHIKLSA-N	C05382
PYR	CHEBI:32816	LCTONWCANYUPML-UHFFFAOYSA-N	C00022
DHAP	CHEBI:16108	GNGACRATGGDKBX-UHFFFAOYSA-N	C00111
AMP		I-KQYNXXCUSA-N	C00020
FBP		I-UYFOZJQFSA-N	C00354
3PG+2PG			C00631
PEP		K-UHFFFAOYSA-M	C00074
6PG	CHEBI:16720	DIRGZFNALBJQ-SQOUGZDYSA-N	C00345
ADP	CHEBI:16761	XTWYTFMLZFPYCI-KQYNXXCUSA-N	C00008
ATP	CHEBI:15422	ZKHQWZAMYRWXGA-KQYNXXCUSA-N	C00002
AcCoA	CHEBI:15351	ZSLZBFCDCINBPY-ZSJKINUSA-N	C00024
F6P	CHEBI:61553	BGWGXPPYQALX-VRPWFDPXSA-N	C00085
Xu5P			C00021
RL			
NA			
NA			
NA			
NADPH	CHEBI:16474	ACFIXIJDZMPPO-NNYOXOHSSA-N	C00005

Double click a rows to load files

File contents is displayed here

Click the bottom to map multiomics data on metabolic network (GML file) after data upload

```
cmd /c perl Mapper.pl transomics_plane_map_withID0125.gml test_multi_omics_a.szf
```

Launch

The gadget require two input files;

(1) **glm** file for blank metabolic pathway map

(e.g., transomics_plane_map_withID0125.gml)

(2) **Shimazu multi-omics dataset** (e.g., test_multi_omics_a.szf)

Sample File:

Sample file to test is available under **Samples > szf**

Requirement: The gadget requires, Anaconda > 2.5.0 (python > 3.5.1)

Multiomics Data Mapper (Output files)

2. Click **Discover** to send data to other gadgets

1. Select whether you want to send the entire **File** or some **Data** to other gadgets

The screenshot shows the Multiomics Data Mapper application window. The 'Output Files' tab is active, displaying a file named 'output.gml'. The main content area shows the GML file's content, which is a VANTED GML file generated with VANTED V2.6.3. The file content includes various settings for a graph, such as colors, grid width, and chart options. At the bottom of the window, there is a command line field containing the command: `cmd /c perl Mapper.pl transomics_plane_map_withID0125.gml test_multi_omics_a.szf` and a 'Launch' button.

```
# generated with VANTED V2.6.3 at Wed Jan 25 17:04:37 JST 2017
graph [
  axis_color "#c0c0c0"
  chart_colors "255,0,0,255:0,0,255;255,255,0,255:0,0,255;0,0,255,255:0,0,255;0,0,255,255:0,0,255;0,255,255,255:"
  connectPriorItems "true"
  graphbackgroundcolor "#ffffff"
  grid_color "#c0c0c0"
  node_axisWidth 1.0
  node_categoryBackgroundColorA "#e1ffff"
  node_categoryBackgroundColorB "#000000"
  node_categoryBackgroundColorC "#ffffe1"
  node_categoryBackgroundColorIndexA -1
  node_categoryBackgroundColorIndexC -1
  node_chartShapeSize 6.0
  node_chartStdDevLineWidth 4.0
  node_chartStdDevTopWidth 10.0
  node_gridWidth 0.5
  node_halfErrorBar "false"
  node_lineChartFillTimeGaps "true"
  node_lineChartShowLines "true"
  node_lineChartShowShapes "true"
  node_lineChartShowStdDev "false"
  node_lineChartShowStdDevRangeLine "true"
  node_outlineBorderWidth 4.0
  node_plotAxisFontSize 30
```

Results Panel

Resultant merged gml is shown in the result panel