

# Shimadzu multi-omics data analysis Tutorial

2017 July

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## Release Date

2017 July

## Contact

For queries, comments and feedback on specific Shimadzu multi-omics analysis gadgets, please mail us at

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For Garuda community gadgets, please send email to

[garudahelp@sbx-corp.com](mailto:garudahelp@sbx-corp.com)

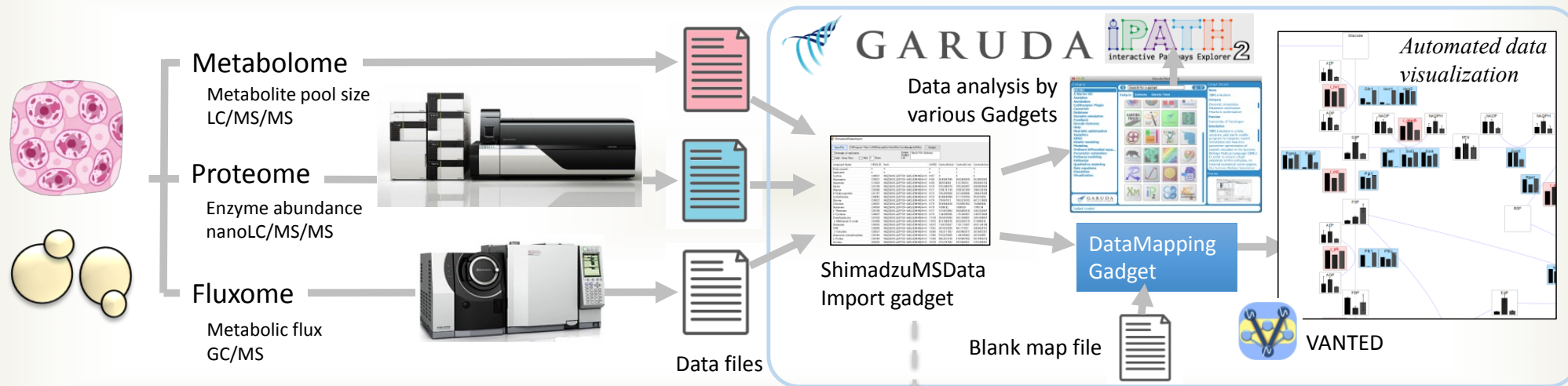
Garuda™

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## What's New ver1.0.1

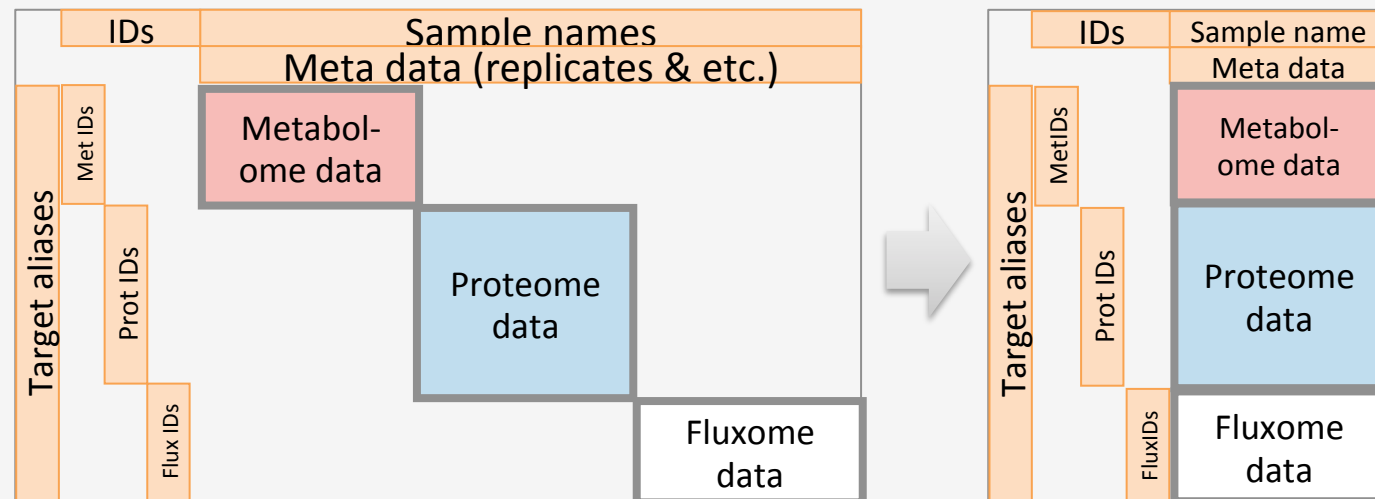
- Shimadzu MSdata Import gadget updated v.1.0.1
  - [File] Add loadable text file format
    - LabSolutions : .txt file
    - LabSolutions Insight : .csv file

# What is the Shimadzu multi-omics data analysis?



**“Shimadzu Multi-Omics Analysis Pack”** can automatically process, analyze proteomics, metabolomics, and flux data obtained by Shimadzu’s gas chromatograph mass spectrometer (GCMS) and liquid chromatography mass spectrometer (LCMS) and visualize the results on pathway maps.

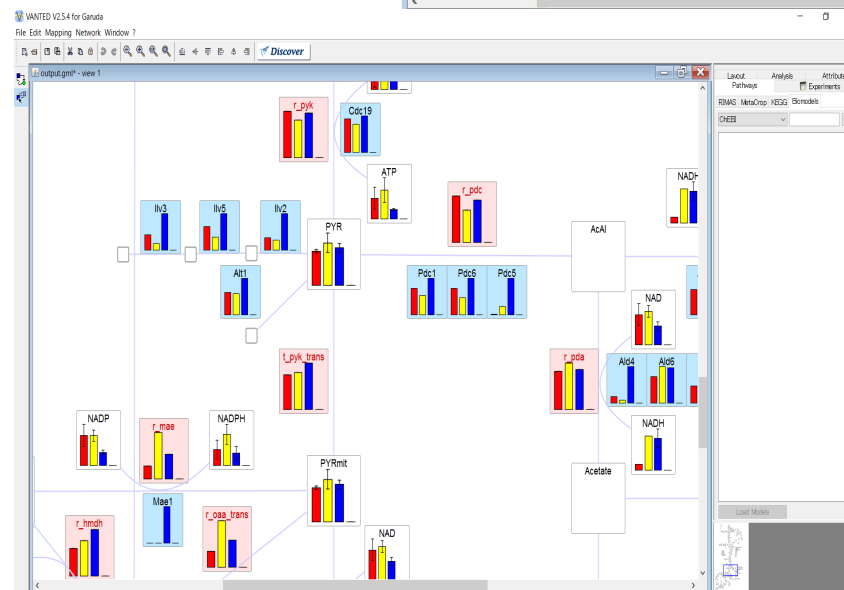
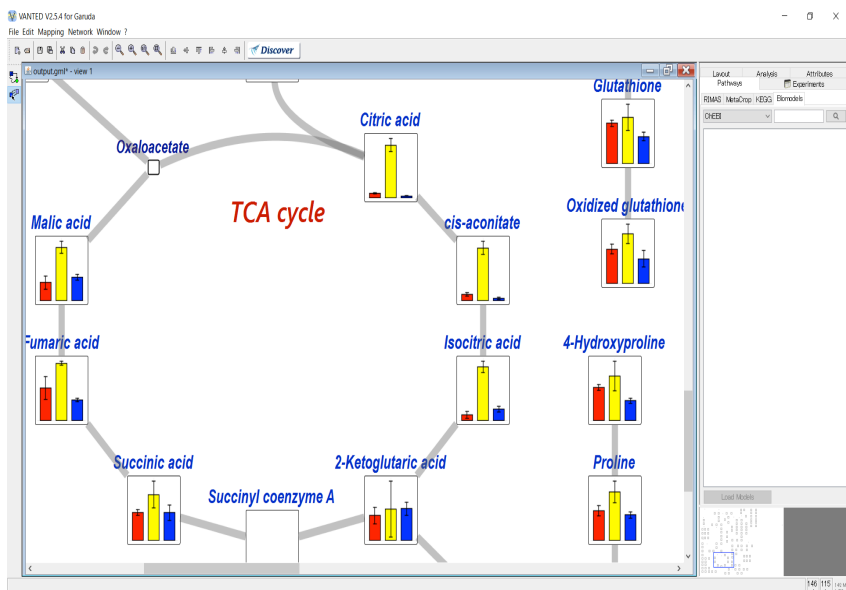
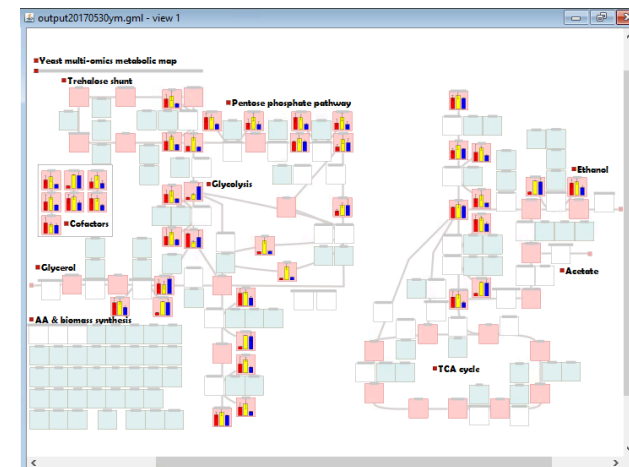
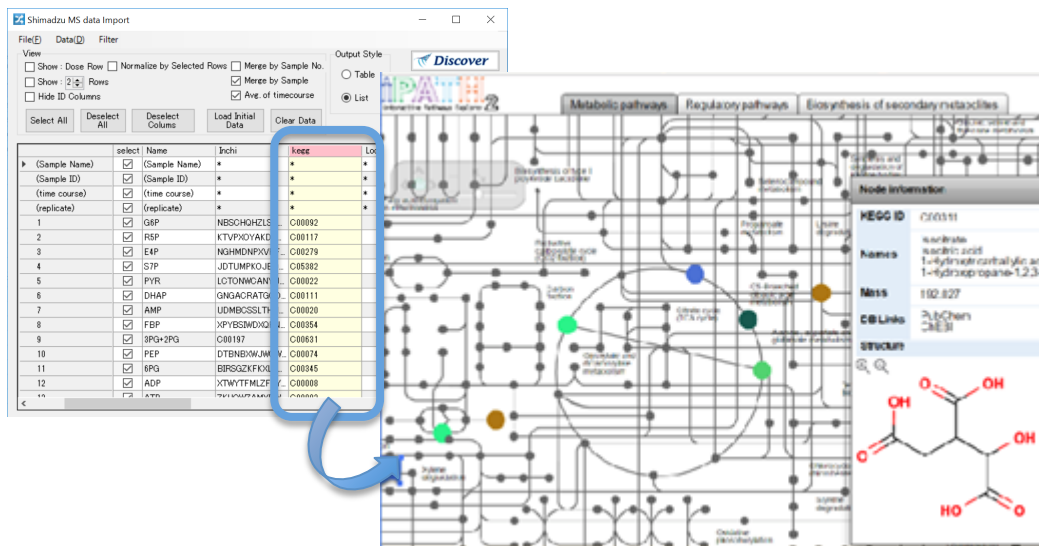
Merge the multi-dimensional data for downstream analytics





# Shimadzu multi-omics analysis visualization

Visualize over pathways  
proteomics, metabolomics, flux data



## Shimadzu Multi-omics Analysis Gadgets

There are 4 gadgets for Shimadzu multi-omics analysis pipeline. The gadgets can format multi-omics data (metabolomics, flux, and proteomics) for downstream analyses and to visualize the data on the pathways / networks.



### Shimadzu MSdata Import

“Shimadzu MSdata Import” gadget can import and merge multi-omics datasets in Shimadzu format for downstream analyses and calculate mean values across replicates for each of the time points.



### Volcano Plot Generator

This gadget generates Volcano Plot Generator visualization and calculates statistics of Volcano Plot Generator analysis from metabolome abundance (lcms) data of Shimadzu.



### Blank GML Generator

This Gadget generates blank .gml file from a list of metabolites and that of associations between the metabolites. A blank .gml file from this gadget will be used as input for “Multiomics Data Mapper” gadget.



### Multiomics Data Mapper

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.



“Shimadzu MSdata Import” gadget can import and merge multi-omics datasets in Shimadzu format for downstream analyses and calculate mean values across replicates for each of the time points.

## INPUT

- Metabolite data
- Proteomics data
- Flux data

(.csv, .txt)

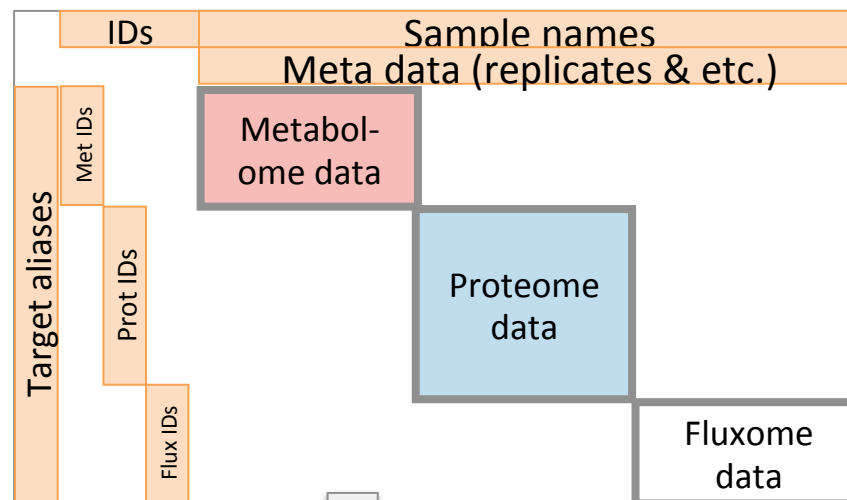


- Merge dataset
- Normalize data
- Average timecourse data
- Imputate data
- Select compounds

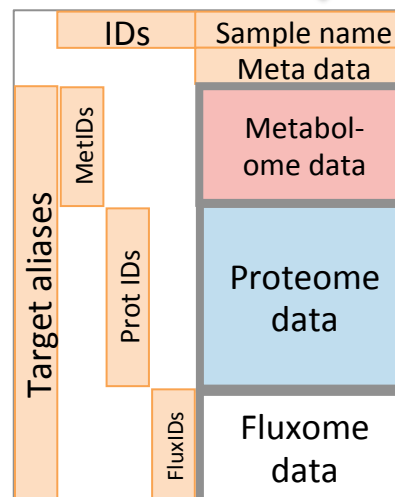
## OUTPUT

- Metabolite data
- Proteomics data
- Flux data
- Mixed data (Metabolite, Proteomics, Flux)
- List of compound ids

(.szf)



Merge dataset





# Volcano Plot Generator

This gadget generates Volcano Plot Generator visualization and calculates statistics of Volcano Plot Generator analysis from metabolome abundance (lcms) data of Shimadzu.

## INPUT

- Metabolite data

(.csv)



- Volcano Plot Generator analysis for metabolome abundance**

## OUTPUT

- Statistics from Volcano Plot Generator analysis
- Metabolome abundance data from Volcano Plot Generator analysis.
- Volcano Plot Generator visualization

(.szf)

Volcano Plot Generator

Input Files Output Files

Discover File Data ?

abundance\_for\_metabolites\_with\_foldchange.szf  
abundance\_for\_metabolites\_with\_foldchange.szf  
abundance\_for\_metabolites\_with\_significance.szf  
abundance\_for\_metabolites\_with\_significance\_and\_foldchange.szf  
log.txt  
statistics\_all.txt  
statistics\_for\_metabolites\_with\_foldchange.txt  
statistics\_for\_metabolites\_with\_significance.txt  
statistics\_for\_metabolites\_with\_significance\_and\_foldchange.txt  
VolcanoPLOT.pdf

Cannot Display File. No Corresponding viewer element.

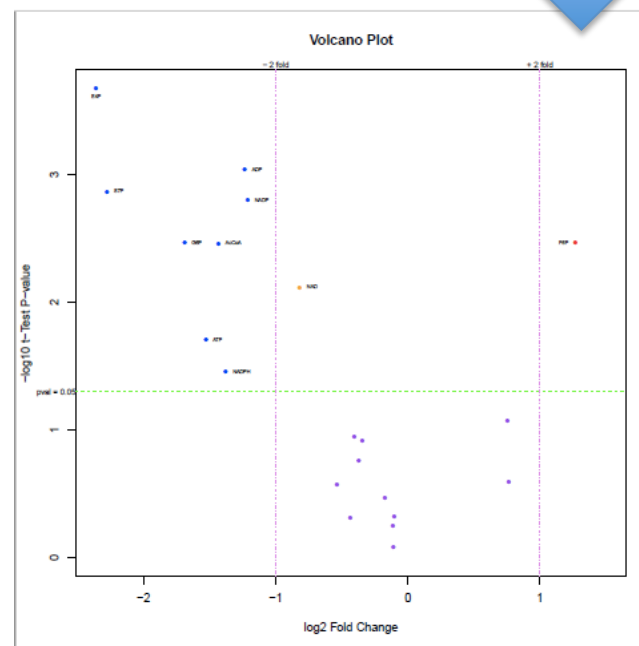
Open in System Editor

Click to see volcano visualization

Double click a row to download files

Launch

Process finished successfully





# Blank GML Generator

This Gadget generates blank .gml file from a list of metabolites and that of associations between the metabolites. A blank .gml file from this gadget will be used as input for “Multiomics Data Mapper” gadget.

## INPUT

- List of Metabolites



- the association between these metabolites

(.csv)

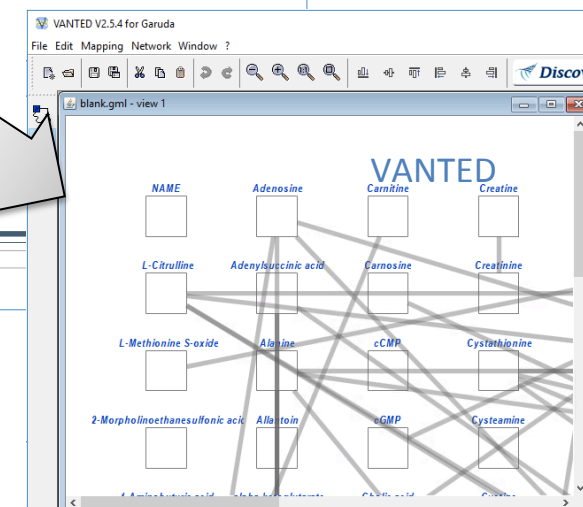
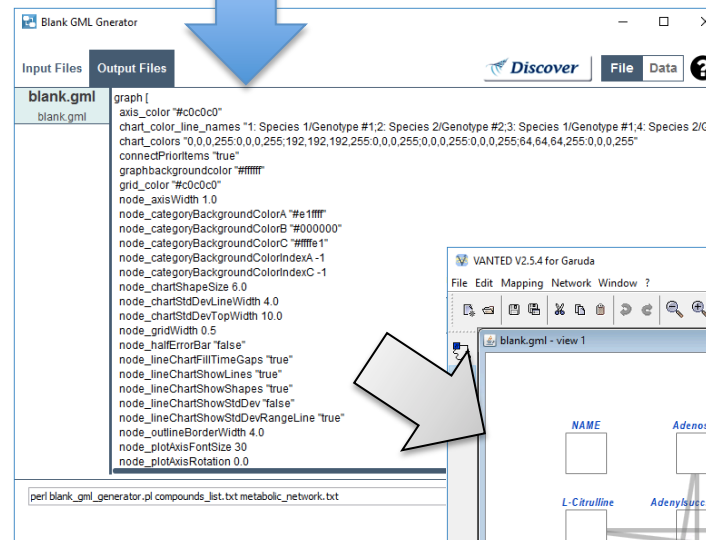
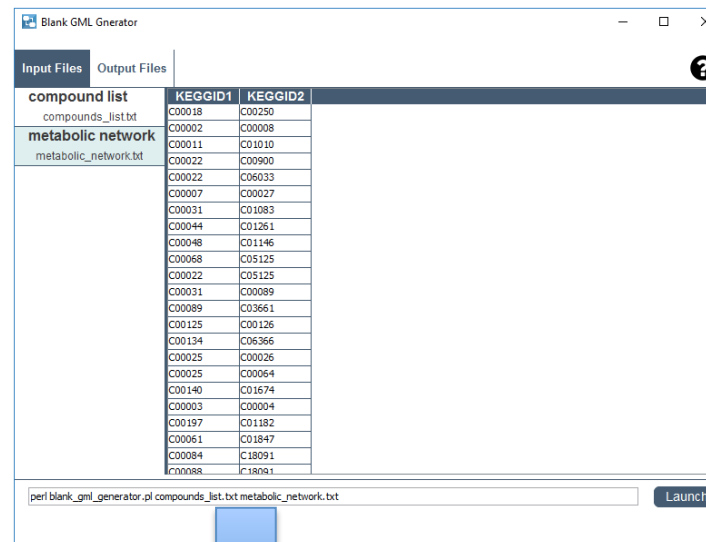


- Generate a blank .gml file for “VANTED”

## OUTPUT

- A blank .gml file  
→ use as an input for Multiomics Data Mapper gadget

(.gml)





# Multiomics Data Mapper

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.

## INPUT

- Merged .szf data output from Shimadzu MSdata Import (.szf)
- .gml file for VANTED (.gml)



- Merge Shimadzu multi-omics data with .gml file for VANTED

## OUTPUT

- Send data to VANTED

(.gml)

Pathway GML File	compound name	ChEBI	Inchi	KEGG COM
transomics_plane_map_withID0125.gml	(Sample No)	*	*	*
Shimadzu Multi-omics Data				
test_multi_omics_a.szf				
	G6P	CHEBI:4170	NBSCHQHZLSJFNQ-GASJEMHNSA-N	C00092
	R5P	CHEBI:52742	KTVPOYAKDPRIY-SOOFDHNSA-N	C00117
	E4P	CHEBI:48153	NGHMDNPXVRFFGS-JUYQGFVSA-N	C00279
	S7P	CHEBI:15721	JDTUMPKOJBQPKX-GBNDHLSA-N	C05382
	PYR	CHEBI:32816	LCTONWCANYUPLM-UHFFFAOYSA-N	C00022
	DHAP	CHEBI:16108	GNACRATGGDKBX-UHFFFAOYSA-N	C00111
	AMP	CHEBI:16027	UDMBCSSLTHHNCB-KQYNOCUSA-N	C00020
	FBP	CHEBI:16905	XPYBSIWDXQFMH-UFOZJQFSA-N	C00354
	3PG+2PG	CHEBI:17835		C00631
	PEP	CHEBI:18021	DTBNBXWJWCWCIC-UHFFFAOYSA-M	C00074
	6PG	CHEBI:48928	BIRSGZKPOLLSJQ-SQOUGZDYSA-N	C00345
	ADP	CHEBI:16761	XTWYTFMLZFPYCI-KQYNOCUSA-N	C00008
	ATP	CHEBI:15422	ZQHQWZAMYRWXGA-KQYNOCUSA-N	C00002
	AcCoA	CHEBI:15351	ZSLZBFCDINBPY-ZSJKINUSA-N	C00024
	F6P	CHEBI:61553	BGWGXPAFYQALX-VRPWFDPKSA-N	C00085
	XuSP			C00231
	RuSP	CHEBI:17363	FNZLVNUWIIPSJ-UHNNWZDZSA-N	C00199
	NAD	CHEBI:15846	BAWFJGJZIEFAR-NNYOXOHSO-O	C00003
	NADP	CHEBI:18009	KJLXINKUBWONI-NNYOXOHSO-O	C00006
	NADH	CHEBI:16908	BOPGDNLQYTO-NNYOXOHSO-O	C00004
	NADPH	CHEBI:16474	ACFIXJJDZMPPD-NNYOXOHSO-O	C00005

cmd /c perl Mapper.pl transomics\_plane\_map\_withID0125.gml test\_multi\_omics\_a.szf

Launch

output.gml

output.gml

# 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;0,255;0;0,255;0;0,255;255;0,0,255;0;0,255;0;0,255;0;0,255;0;0,255;0;0,255;255;255;"
  connectedPriorItems "true"
  graphbackgroundcolor "#ffffff"
  grid_color "#c0c0c0"
  node_axisWidth 1.0
  node_categoryBackgroundColorA "#e1fff1"
  node_categoryBackgroundColorB "#000000"
  node_categoryBackgroundColorC "#ffffff"
  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
]
```

cmd /c perl Mapper.pl transomics\_plane\_map\_withID0125.gml test\_multi\_omics\_a.szf

VANTED

VANTED visualization showing a metabolic pathway map with various metabolites and their associated data points.

# Installation and Troubleshooting

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## Gadget's dependency information

- **“Volcano Plot Generator”** gadget requires several **R packages**, “limma”, “pcaMethods”, “crmn”, and “metabolomics” packages. The gadget automatically install the packages in your computer, if the gadgets were not installed in your computer.
- **“Volcano Plot Generator”** gadget requires **R language** > 3.2.2. Please follow the instruction document ([How to install R.pdf](#)).
- **“Multiomics Data Mapper”** gadget requires, **Anaconda** > 2.5.0 (python > 3.5.1), a distribution of python language. Please follow the instruction document ([How to install Python.pdf](#)).

## Shimadzu Gadgets -Troubleshooting

- In case of incorrect inputs, it will show a red text in bottom of the gadget window for incorrect input
- You can edit the command in the command line to the left of Launch command
- In this release, if the gadget fails, the gadget will not close (recommend to add the following to the launch command – cmd /c start)
- Output files should be sent to Nandi by Discover button to export them locally.
- Shimadzu metabolome analysis gadgets can be connected in a manual pipeline for building an analytics pipeline. Tutorial coming soon!

# Introduction of Gadgets

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**Shimadzu MSdata Import**



**Volcano Plot Generator**



**Blank GML Generator**



**Multiomics Data Mapper**



“Shimadzu MSdata Import” gadget can import and merge multi-omics datasets in Shimadzu format for downstream analyses and calculate mean values across replicates for each of the time points.

## INPUT

- Metabolite data
- Proteomics data
- Flux data

**(.csv, .txt)**

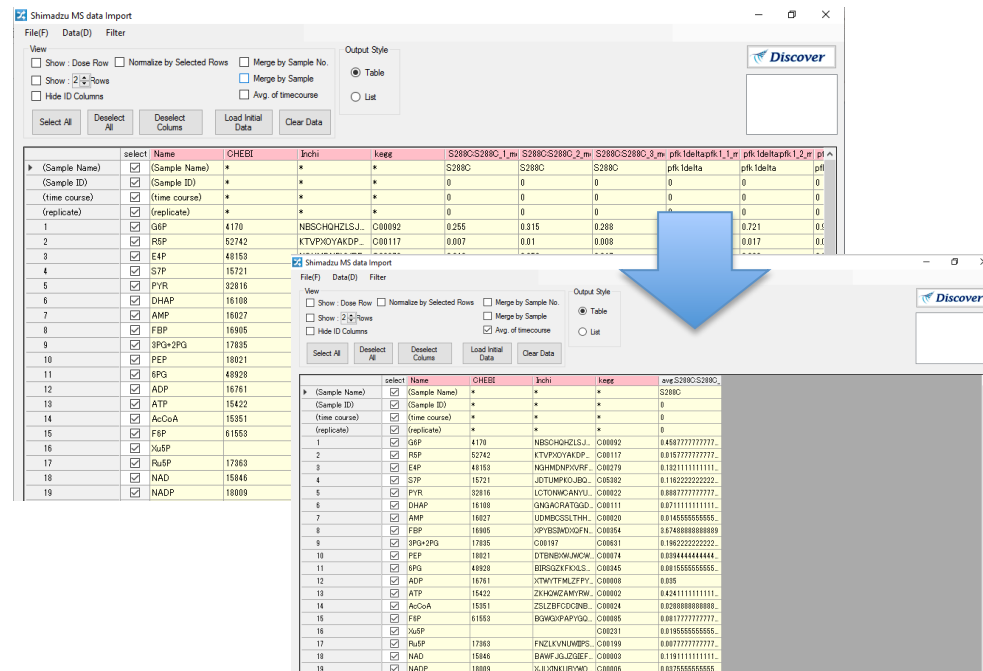
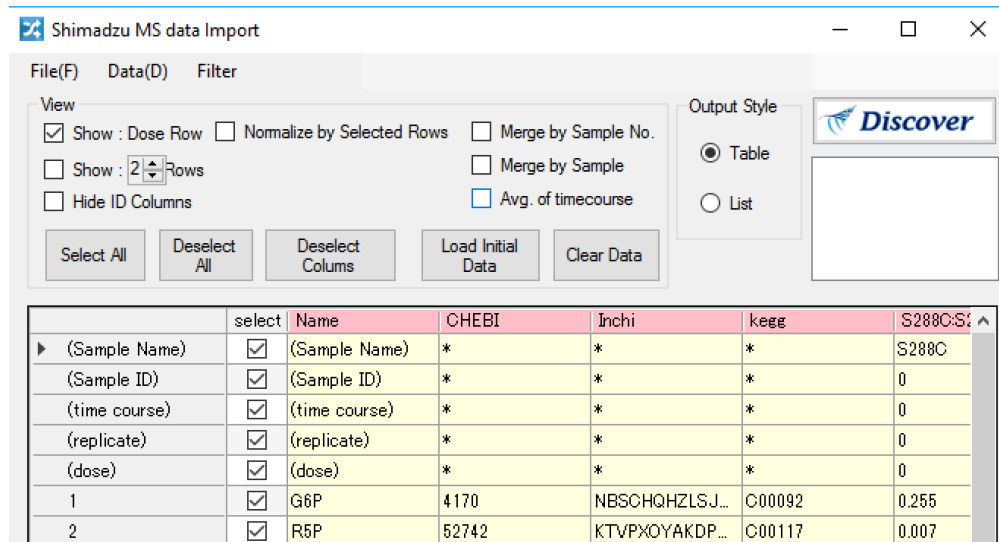


- **Clear Load Data**
- **Edit Data**
- **Imputate data**
- **Average timecourse data**
- **Merge dataset**
- **Select Output Style**

## OUTPUT

- Metabolite data
- Proteomics data
- Flux data
- Mixed data (Metabolite, Proteomics, Flux)
- List of compound ids

**(.szf)**





## PREPARE INPUT DATA

- LabSolutions (.txt)
- LabSolutions Insight (.csv, .txt)

## INPUT

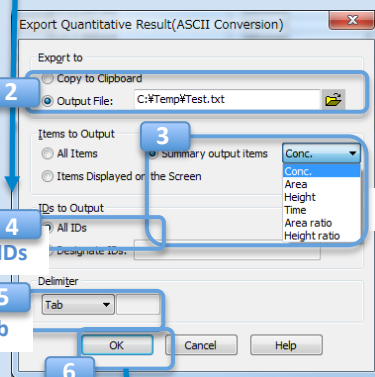
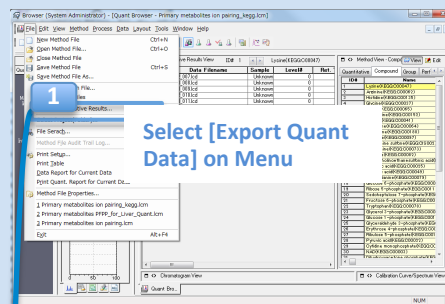
- Metabolite data
- Proteomics data
- Flux data

(.csv, .txt)

You can prepare the input data for Shimadzu MSdata Import gadget from LabSolutions / LabSolutions Insight.

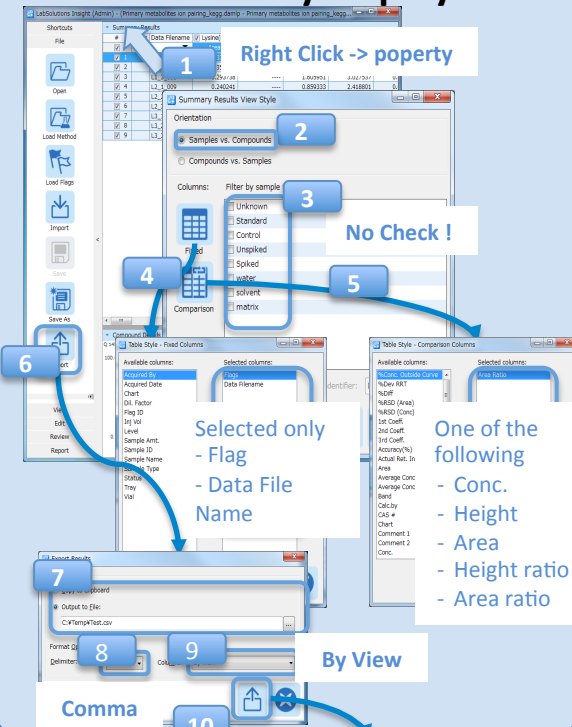
## Shimadzu MS data (.lcb or .lcm and .lcd)

### LabSolutions - Quant browser



.txt

### LabSolutions Insight - Summary display



.CS



Shimadzu MSdata Import



## INPUT

- Metabolite data
- Proteomics data
- Flux data

(.csv, .txt)

### 1. Click to select, load, and merge multi-omics data files

- “Add Protein quant”
- “Add Metabolite quant”
- “Add Flux quant”

to select data files for protein abundance, metabolome abundance, flux, respectively).

**Note:** if you select and load two different data files, the gadget merges the two selected files to make a single data table.

**Note:** Loadable columns < about 650 columns

**Sample File:** Sample file to test is available under ShimadzuGadgets\_SampleData > ShimadzuMSdataImport

The gadget can import and merge data files for metabolome abundance, proteome abundance, and flux (e.g., Sample\_multi\_omics\_metabolome\_data.csv, Sample\_multi\_omics\_proteome\_data.csv, and Sample\_multi\_omics\_metabolic\_flux.csv, respectively).

Click to select, load, and merge multi-omics data files

A imported data table is displayed here

	select	Name	CHEBI	Inchi	kegg	S288C-S288C_1_mv	S288C-S288C_2_mv	S288C-S288C_3_mv	pfk1delta	pfk1_1_mv	pfk1c
(Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	S288C	S288C	S288C	0	0	0
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0	0	0	0	0	0
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	0	0	0	0	0	0
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	0	0	0	0	0	0
1	<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLSJ...	C00092	0.255	0.315	0.288	0.813	0.721	
2	<input checked="" type="checkbox"/>	R5P	52742	KTVXPXOYAKDP...	C00117	0.007	0.01	0.008	0.022	0.017	
3	<input checked="" type="checkbox"/>	E4P	48153	NGHMDNPXVRF...	C00279	0.046	0.053	0.047	0.263	0.263	
4	<input checked="" type="checkbox"/>	S7P	15721	JDTUMPKOJBQ...	C05382	0.029	0.038	0.032	0.234	0.24	
5	<input checked="" type="checkbox"/>	PYR	32816	LCTONWCANYU...	C00022	0.806	0.825	0.763	1.092	0.812	
6	<input checked="" type="checkbox"/>	DHAP	16108	GNGACRATGGD...	C00111	0.042	0.081	0.068	0.054	0.041	
7	<input checked="" type="checkbox"/>	AMP	16027	UIMBOSSTH...	C00030	0.022	0.017	0.01	0.015	0.015	
8	<input checked="" type="checkbox"/>	FBP	11						1.916	1.755	
9	<input checked="" type="checkbox"/>	3PG+2PG	1						0.201	0.206	
10	<input checked="" type="checkbox"/>	PEP	18021	DTBNBXWJWCW...	C00074	0.029	0.038	0.026	0.043	0.046	
11	<input checked="" type="checkbox"/>	6PG	48928	BIRSGZKFKXLS...	C00345	0.073	0.075	0.073	0.092	0.078	
12	<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY...	C00008	0.012	0.054	0.034	0.053	0.044	
13	<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW...	C00002	0.399	0.633	0.313	0.609	0.434	
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFCDGIB...	C00024	0.028	0.045	0.024	0.043	0.031	
15	<input checked="" type="checkbox"/>	F6P	61553	BGWGXPAFYGQ...	C00085	0.031	0.025	0.03	0.061	0.058	
16	<input checked="" type="checkbox"/>	Xu5P			C00231	0.008	0.013	0.012	0.023	0.02	
17	<input checked="" type="checkbox"/>	Ru5P	17363	FNZLKVNUWIPS...	C00199	0.002	0.005	0.005	0.012	0.008	
18	<input checked="" type="checkbox"/>	NAD	15846	BAWFJGJZGIEF...	C00003	0.112	0.169	0.112	0.144	0.162	
19	<input checked="" type="checkbox"/>	NADP	16008	YHUKYKIPY...	C00006	0.043	0.06	0.037	0.047	0.04	



## Data Processing

- Clear Load Data
- Edit Data
- Impute data
- Average timecourse data
- Merge dataset
- Select Output Style

1. Select **“Clear Load Data”** to clear the data uploaded on the gadget.

Shimadzu MS data Import

File(F) Data(D) Filter

View

☐ Show : Dose Row ☐ Normalize by Selected Rows ☐ Merge by Sample No.

☐ Show : 2 Rows ☐ Merge by Sample

☐ Hide ID Columns ☐ Avg. of timecourse

Output Style

☒ Table

☐ List

Select All Deselect All Deselect Columns Load Initial Data Clear Data

	select	Name	CHEBI	Inchi	kegg	S288C-S288C_1_m	S288C-S288C_2_m	S288C-S288C_3_m	pkf1delta	pkf1_1_r	pkf1c
(Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	S288C	S288C	S288C	pkf1delta	pkf1c	
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0	0	0	0	0	
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	0	0	0	0	0	
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	0	0	0	0	0	
1	<input checked="" type="checkbox"/>	G6P	4170						0.813	0.721	
2	<input checked="" type="checkbox"/>	R5P	52742						0.022	0.017	
3	<input checked="" type="checkbox"/>	E4P	48153						0.263	0.263	
4	<input checked="" type="checkbox"/>	S7P	15721	JDUMPKOJBQ...	C00382	0.029	0.038	0.032	0.234	0.24	
5	<input checked="" type="checkbox"/>	PYP	32816	LCTONWCANYU...	C00022	0.806	0.825	0.763	1.092	0.812	
6	<input checked="" type="checkbox"/>	DHAP	16108	GNGACRATGGD...	C00111	0.042	0.081	0.068	0.054	0.041	
7	<input checked="" type="checkbox"/>	AMP	16027	UDMBCSSLTHH...	C00020	0.023	0.017	0.01	0.015	0.015	
8	<input checked="" type="checkbox"/>	FBP	16905	XPYBSIWDXQFN...	C00354	5.428	5.214	4.981	1.916	1.755	
9	<input checked="" type="checkbox"/>	3PG+2PG	17835	C00197	C00631	0.164	0.225	0.17	0.201	0.206	
10	<input checked="" type="checkbox"/>	PEP	18021	DTBNBXWJWCW...	C00074	0.029	0.038	0.026	0.043	0.046	
11	<input checked="" type="checkbox"/>	6PG	48928	BIPSGZKFKXLS...	C00345	0.073	0.075	0.073	0.092	0.078	
12	<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY...	C00008	0.012	0.054	0.034	0.053	0.044	
13	<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW...	C00002	0.399	0.633	0.313	0.609	0.434	
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFDCINB...	C00024	0.028	0.045	0.024	0.043	0.031	
15	<input checked="" type="checkbox"/>	F6P	61553	BGWSXPAPYQG...	C00085	0.031	0.025	0.03	0.061	0.058	
16	<input checked="" type="checkbox"/>	Xu5P		C00231	C00231	0.008	0.013	0.012	0.023	0.02	
17	<input checked="" type="checkbox"/>	Ru5P	17363	FNZLKVNUWIPS...	C00199	0.002	0.005	0.005	0.012	0.008	
18	<input checked="" type="checkbox"/>	NAD	15846	BAWFJGJZGIEF...	C00003	0.112	0.169	0.112	0.144	0.162	

Click “Clear Load Data” to clear the data uploaded on the gadget

Shimadzu MS data Import

File(F) Data(D) Filter

View

☐ Show : Dose Row ☐ Normalize by Selected Rows ☐ Merge by Sample No.

☐ Show : 2 Rows ☐ Merge by Sample

☐ Hide ID Columns ☐ Avg. of timecourse

Output Style

☒ Table

☐ List

Select All Deselect All Deselect Columns Load Initial Data Clear Data



## Data Processing

- Clear Load Data
- **Edit Data**
- Impute data
- Average timecourse data
- Merge dataset
- Select Output Style

1. Select cells to edit the data in the cells.

Shimadzu MS data Import

File Data Filter

View

☐ Show : Dose Row ☐ Normalize by Selected Rows ☐ Merge by Sample No.

☐ Show : 2 Rows ☐ Merge by Sample

☐ Hide ID Columns ☐ Avg. of timecourse

Output Style

☒ Table ☐ List

Select All Deselect All Deselect Columns Load Initial Data Clear Data

	select	Name	CHEBI	Inchi	kegg	S288C	S288C	S288C	pkf Idelta	pkf Idelta
(Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	0	0	0	0	0
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0	0	0	0	0
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	0	0	0	0	0
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	0	0	0	0	0
1	<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLSJ...	C00092	0.255	0.315	0.288	0.813	0
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPOYAKDP...	C00117	0.007	0.01	0.008	0.022	0
3	<input checked="" type="checkbox"/>	E4P	48153	NGHMDNPVRF...	C00279	0.046	0.053	0.047	0.263	0
4	<input checked="" type="checkbox"/>	S7P	15721	JDTUMPKOJBQ...	C05382	0.029	0.038	0.032	0.234	0
5	<input checked="" type="checkbox"/>	PYR	32816	LOTONWCANYU...	C00022	0.806	0.825	0.763	1.092	0
6	<input checked="" type="checkbox"/>	DHAP	16108	GNGACRATGG...	C00111	0.042	0.081	0.068	0.054	0
7	<input checked="" type="checkbox"/>	AMP	16027	UOMBSCSLTHH...	C00020	0.023	0.017	0.01	0.015	0
8	<input checked="" type="checkbox"/>	FBP	16905	XPYBSMDXQFN...	C00354	5.428	5.214	4.981	1.916	1
9	<input checked="" type="checkbox"/>	3PG+2PG	17835	C00197	C00631	0.164	0.225	0.17	0.201	0
10	<input checked="" type="checkbox"/>	PEP	18021	DTENBXWJMCW...	C00074	0.029	0.038	0.026	0.043	0
11	<input checked="" type="checkbox"/>	6PG	48928	BIRSGZKFKLS...	C00345	0.073	0.075	0.073	0.092	0
12	<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY...	C00008	0.012	0.054	0.034	0.053	0
13	<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW...	C00002	0.399	0.633	0.313	0.609	0
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFDCINB...	C00024	0.028	0.045	0.024	0.043	0
15	<input checked="" type="checkbox"/>	F6P	61553	BGWGXPAFYGO...	C00085	0.031	0.025	0.03	0.061	0
16	<input checked="" type="checkbox"/>	Xu5P			C00231	0.008	0.013	0.012	0.023	0

Select cells to edit the data in the cells

Shimadzu MS data Import

File Data Filter

View

☐ Show : Dose Row ☐ Normalize by Selected Rows ☐ Merge by Sample No.

☐ Show : 2 Rows ☐ Merge by Sample

☐ Hide ID Columns ☐ Avg. of timecourse

Output Style

☒ Table ☐ List

Select All Deselect All Deselect Columns Load Initial Data Clear Data

	select	Name	CHEBI	Inchi	kegg	S288C	S288C	S288C	pkf Idelta	pkf Idelta
(Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	0	0	0	0	0
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0	0	0	0	0
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	1	1	1	2	0
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	0	0	0	0	0
1	<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLSJ...	C00092	0.255	0.315	0.288	0.813	0
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPOYAKDP...	C00117	0.007	0.01	0.008	0.022	0
3	<input checked="" type="checkbox"/>	E4P	48153	NGHMDNPVRF...	C00279	0.046	0.053	0.047	0.263	0
4	<input checked="" type="checkbox"/>	S7P	15721	JDTUMPKOJBQ...	C05382	0.029	0.038	0.032	0.234	0
5	<input checked="" type="checkbox"/>	PYR	32816	LOTONWCANYU...	C00022	0.806	0.825	0.763	1.092	0
6	<input checked="" type="checkbox"/>	DHAP	16108	GNGACRATGG...	C00111	0.042	0.081	0.068	0.054	0
7	<input checked="" type="checkbox"/>	AMP	16027	UOMBSCSLTHH...	C00020	0.023	0.017	0.01	0.015	0
8	<input checked="" type="checkbox"/>	FBP	16905	XPYBSMDXQFN...	C00354	5.428	5.214	4.981	1.916	1
9	<input checked="" type="checkbox"/>	3PG+2PG	17835	C00197	C00631	0.164	0.225	0.17	0.201	0
10	<input checked="" type="checkbox"/>	PEP	18021	DTENBXWJMCW...	C00074	0.029	0.038	0.026	0.043	0
11	<input checked="" type="checkbox"/>	6PG	48928	BIRSGZKFKLS...	C00345	0.073	0.075	0.073	0.092	0
12	<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY...	C00008	0.012	0.054	0.034	0.053	0
13	<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW...	C00002	0.399	0.633	0.313	0.609	0
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFDCINB...	C00024	0.028	0.045	0.024	0.043	0
15	<input checked="" type="checkbox"/>	F6P	61553	BGWGXPAFYGO...	C00085	0.031	0.025	0.03	0.061	0
16	<input checked="" type="checkbox"/>	Xu5P			C00231	0.008	0.013	0.012	0.023	0

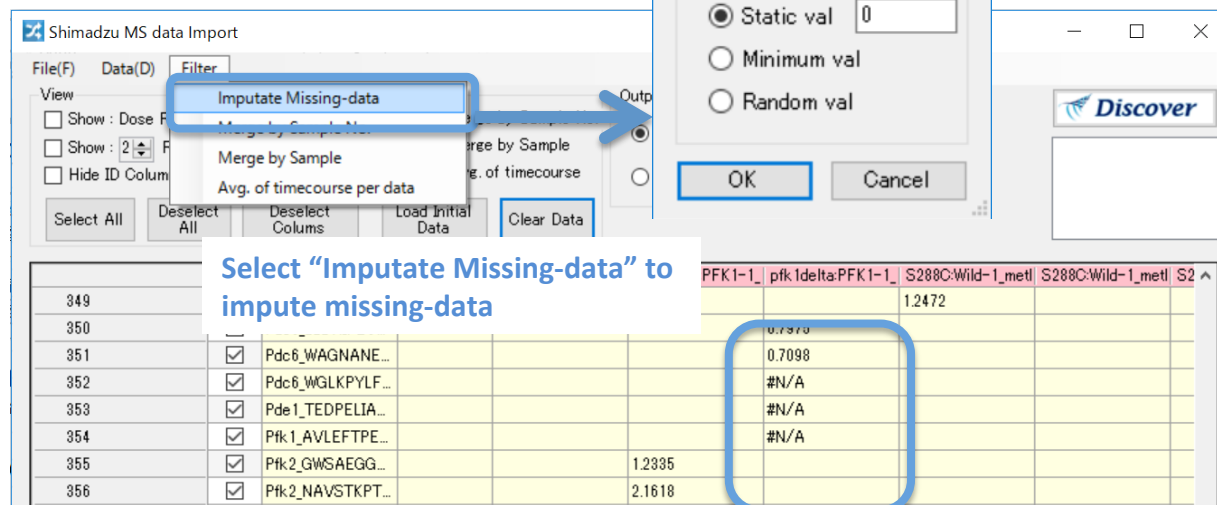


## Data Processing

- Clear Load Data
- Edit Data
- **Impute data**
- Average timecourse data
- Merge dataset
- Select Output Style

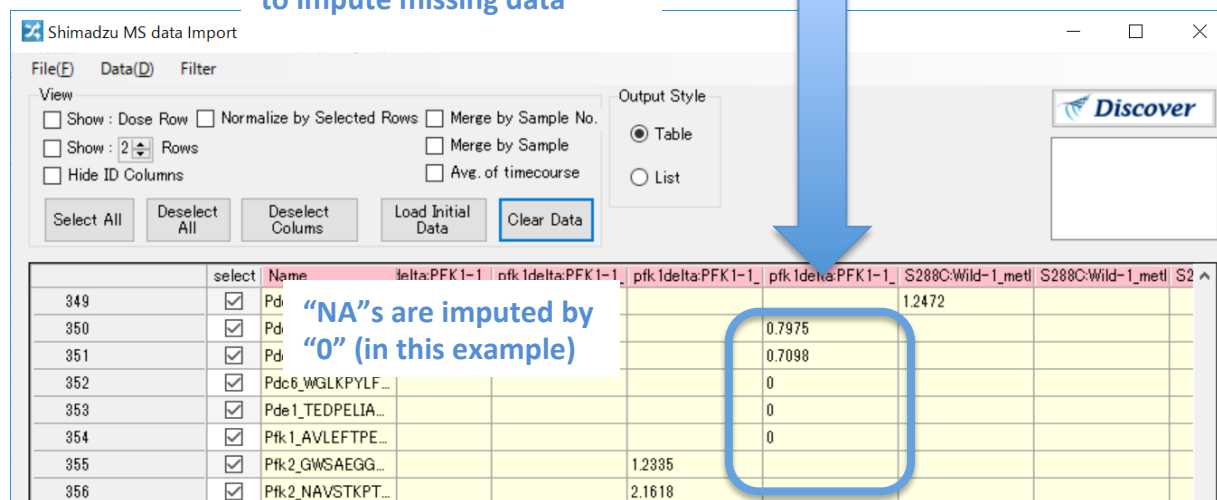
1. Select **"Impute Missing-data"** to impute missing-data (e.g., NA) in the imported omics data. By clicking the button, a window (see dialog ②) comes up.
2. **"All data"** and **"Selected"** indicate target data cells (all cells and selected cell respectively) to impute missing-data.  
**"Static val"**,  
**"Minimum val"**, and  
**"Random val"**,  
indicate a value (user defined value, minimum value in the data, value selected randomly from the data, respectively) that are used to impute missing-data.
3. After the setting, click **"OK"** to impute missing data.

**"All data"** and **"Selected"** indicate target data cells to impute missing-data



Select **"Impute Missing-data"** to impute missing-data

After the setting, click **"OK"** to impute missing data

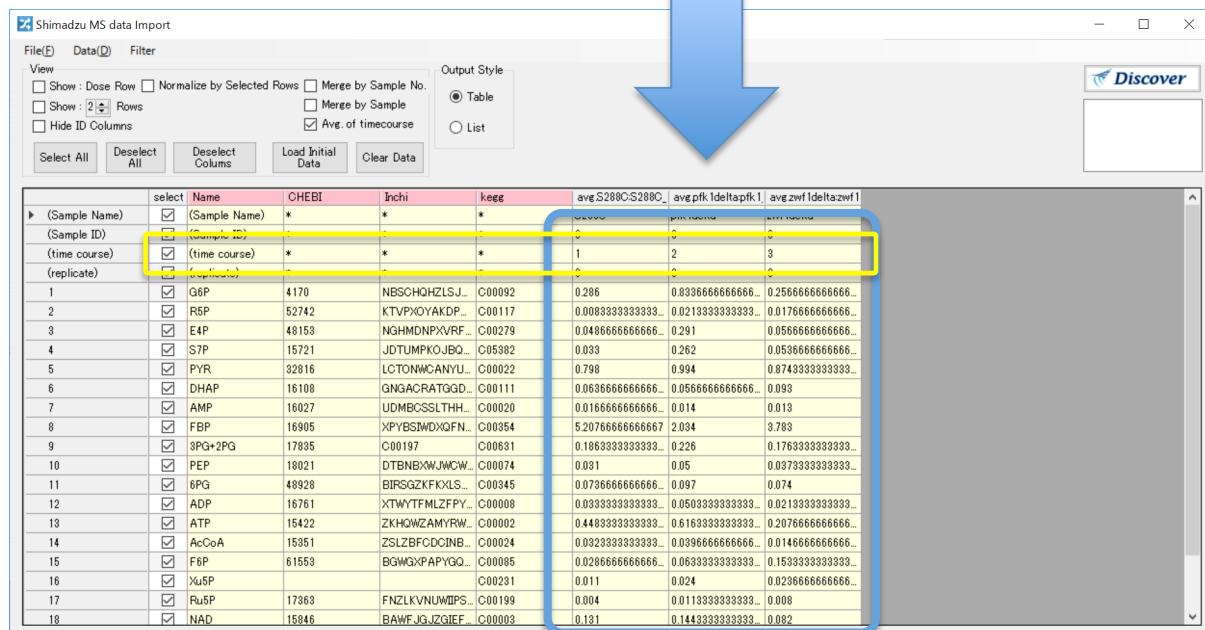


**"NA"s are imputed by  
"0" (in this example)**



- Clear Load Data
- Edit Data
- Impute data
- **Average timecourse data**
- Merge dataset
- Select Output Style

1. Click check box of “**Average of Time course per data**” to calculate mean value (e.g.,. Mean value for metabolome abundance, proteome abundance, and flux) among replicates for each of the time points.







## Data Processing

- Clear Load Data
- Edit Data
- Impute data
- Average timecourse data
- **Merge dataset**
- Select Output Style

1. Click check box of “**Merge by Sample**” to merge columns using a common sample name.

Shimadzu MS data Import

File(F) Data(D) Filter

View

☐ Show : Dose Row ☐ Normalize by Selected Rows ☐ Merge by Sample No. ☒ Merge by Sample ☐ Avg. of timecourse

☐ Show : 2 Rows ☐ Hide ID Columns

Output Style

☒ Table ☐ List

Select All Deselect All Deselect Columns Load Initial Data Clear Data

(Sample Name)	(Sample ID)	(time course)	(replicate)	G6P	R5P	E4P	S7P	PYR	DHAP	AMP	FBP	3PG+2PG	PEP	6PG	ADP	ATP	AcCoA	F6P	Xu5P	Ru5P
1	2	3	4	5	6	7	8	9	0	0	0	0	0	0	0	0	0	0	0	0
0.286	0.8336666666666666	0.2566666666666666	0.008333333333333333	0.02133333333333333	0.01766666666666666	0.04866666666666666	0.291	0.05666666666666666	0.033	0.262	0.05366666666666666	0.798	0.994	0.8743333333333333	0.06366666666666666	0.05666666666666666	0.093	0.01666666666666666	0.014	0.013
5.207666666666667	2.034	3.783	0.1863333333333333	0.226	0.1763333333333333	0.031	0.05	0.03733333333333333	0.07366666666666666	0.097	0.074	0.03333333333333333	0.05033333333333333	0.02133333333333333	0.4483333333333333	0.6163333333333333	0.2076666666666666	0.03233333333333333	0.03966666666666666	0.01466666666666666
0.02866666666666666	0.06333333333333333	0.1533333333333333	0.011	0.024	0.02366666666666666	0.004	0.01133333333333333	0.008												

Click check box of “Merge by Sample” to merge columns using a common sample name

Shimadzu MS data Import

File(F) Data(D) Filter

View

☐ Show : Dose Row ☐ Normalize by Selected Rows ☐ Merge by Sample No. ☒ Merge by Sample ☒ Avg. of timecourse

☐ Show : 2 Rows ☐ Hide ID Columns

Output Style

☒ Table ☐ List

Select All Deselect All Deselect Columns Load Initial Data Clear Data

(Sample Name)	(Sample ID)	(time course)	(replicate)	G6P	R5P	E4P	S7P	PYR	DHAP	AMP	FBP	3PG+2PG	PEP	6PG	ADP	ATP	AcCoA	F6P	Xu5P	Ru5P
1	2	3	4	5	6	7	8	9	0	0	0	0	0	0	0	0	0	0	0	0
0.286	0.8336666666666666	0.2566666666666666	0.008333333333333333	0.02133333333333333	0.01766666666666666	0.04866666666666666	0.291	0.05666666666666666	0.033	0.262	0.05366666666666666	0.798	0.994	0.8743333333333333	0.06366666666666666	0.05666666666666666	0.093	0.01666666666666666	0.014	0.013
5.207666666666667	2.034	3.783	0.1863333333333333	0.226	0.1763333333333333	0.031	0.05	0.03733333333333333	0.07366666666666666	0.097	0.074	0.03333333333333333	0.05033333333333333	0.02133333333333333	0.4483333333333333	0.6163333333333333	0.2076666666666666	0.03233333333333333	0.03966666666666666	0.01466666666666666
0.02866666666666666	0.06333333333333333	0.1533333333333333	0.011	0.024	0.02366666666666666	0.004	0.01133333333333333	0.008												





## Data Processing

- Clear Load Data
- Edit Data
- Impute data
- Average timecourse data
- Merge dataset
- **Select Output Style**

1. Click “List” at “Output Style” to output list of compound ids.
2. Enter the “kegg” column.

Click “List” at “Output Style” to output list of compound ids

Enter the “kegg” column

	select	Name	CHEBI	Inchi	kegg	Loc us id	Peptide	Prefered name	UniProt
(Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	*	*	*	*
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	*	*	*	*
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	*	*	*	*
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	*	*	*	*
1	<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLS...	C00092				
2	<input checked="" type="checkbox"/>	R5P	52742	KTVXPYOYAKDP...	C00117				
3	<input checked="" type="checkbox"/>	E4P	48153	NGHMDNPXVRF...	C00279				
4	<input checked="" type="checkbox"/>	S7P	15721	JDTUMPKOJBQ...	C05382				
5	<input checked="" type="checkbox"/>	PYR	32816	LCTONWCANYU...	C00022				
6	<input checked="" type="checkbox"/>	DHAP	16108	GNGACRATGGD...	C00111				
7	<input checked="" type="checkbox"/>	AMP	16027	UDMBCSSLTHH...	C00020				
8	<input checked="" type="checkbox"/>	FBP	16905	XPYBSIWDXQFN...	C00354				
9	<input checked="" type="checkbox"/>	3PG+2PG	17835	C00197	C00631				
10	<input checked="" type="checkbox"/>	PEP	18021	DTBNBXWJWCW...	C00074				
11	<input checked="" type="checkbox"/>	6PG	48928	BIRSGZKFKXLS...	C00345				
12	<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY...	C00008				
13	<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW...	C00002				
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFDCINB...	C00024				
15	<input checked="" type="checkbox"/>	F6P	61553	BGWGXPPAPYG...	C00085				

Discover

	select	Name	CHEBI	Inchi	kegg	Loc us id	Peptide	Prefered name	UniProt
▶ (Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	*	*	*	*
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	*	*	*	*
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	*	*	*	*
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	*	*	*	*
1	<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLS...	C00092				
2	<input checked="" type="checkbox"/>	R5P	52742	KTVXPYOYAKDP...	C00117				
3	<input checked="" type="checkbox"/>	E4P	48153	NGHMDNPXVRF...	C00279				
4	<input checked="" type="checkbox"/>	S7P	15721	JDTUMPKOJBQ...	C05382				
5	<input checked="" type="checkbox"/>	PYR	32816	LCTONWCANYU...	C00022				
6	<input checked="" type="checkbox"/>	DHAP	16108	GNGACRATGGD...	C00111				
7	<input checked="" type="checkbox"/>	AMP	16027	UDMBCSSLTHH...	C00020				
8	<input checked="" type="checkbox"/>	FBP	16905	XPYBSIWDXQFN...	C00354				
9	<input checked="" type="checkbox"/>	3PG+2PG	17835	C00197	C00631				
10	<input checked="" type="checkbox"/>	PEP	18021	DTBNBXWJWCW...	C00074				
11	<input checked="" type="checkbox"/>	6PG	48928	BIRSGZKFKXLS...	C00345				
12	<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY...	C00008				
13	<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW...	C00002				
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFDCINB...	C00024				
15	<input checked="" type="checkbox"/>	F6P	61553	BGWGXPPAPYG...	C00085				



## OUTPUT

- Metabolite data
- Proteomics data
- Flux data
- Mixed data (Metabolite, Proteomics, Flux)
- List of compound ids

(.szf)

1. Click “**Discover**” to list up downstream analysis gadgets that can handle the data imported (merged) in **Shimadzu MSdata Import**.
2. Select and double click the **gadget** to send the imported (merged) data to the gadget.

Click “Discover” to list up downstream analysis gadgets

Select and double click the gadget to send the imported data to the gadget

	select	Name	peptide	Preferred name	UniProt	map1	map2	map3
(Sample Name)	<input checked="" type="checkbox"/>	(Sample I						*
(Sample ID)	<input checked="" type="checkbox"/>	(Sample II						*
▶ (time course)	<input checked="" type="checkbox"/>	(time cour						*
(replicate)	<input checked="" type="checkbox"/>	(replicate)						*
1	<input checked="" type="checkbox"/>	G6P						
2	<input checked="" type="checkbox"/>	R5P						
3	<input checked="" type="checkbox"/>	E4P						
4	<input checked="" type="checkbox"/>	S7P						
5	<input checked="" type="checkbox"/>	PYR						
6	<input checked="" type="checkbox"/>	DHAP						
7	<input checked="" type="checkbox"/>	AMP						
8	<input checked="" type="checkbox"/>	FBP						
9	<input checked="" type="checkbox"/>	3PG+2PG						
10	<input checked="" type="checkbox"/>	PEP						
11	<input checked="" type="checkbox"/>	6PG						
12	<input checked="" type="checkbox"/>	ADP						
13	<input checked="" type="checkbox"/>	ATP						
14	<input checked="" type="checkbox"/>	AcCoA						



# Volcano Plot Generator

This gadget generates Volcano Plot Generator visualization and calculates statistics of Volcano Plot Generator analysis from metabolome abundance (lcms) data of Shimadzu.

## INPUT

- Metabolite data

(.csv)



- Volcano Plot Generator analysis for metabolome abundance**

## OUTPUT

- Statistics from Volcano Plot Generator analysis
- Metabolome abundance data from Volcano Plot Generator analysis.
- Volcano Plot Generator visualization

(.szf)

Volcano Plot Generator

Input Files Output Files

Discover File Data ?

abundance_for_metabolites_with_foldchange.szf	abundance_for_metabolites_with_foldchange.szf
abundance_for_metabolites_with_significance.szf	abundance_for_metabolites_with_significance.szf
abundance_for_metabolites_with_significance_and_foldchange.szf	abundance_for_metabolites_with_significance_and_foldchange.szf
log.txt	log.txt
statistics_all.txt	statistics_all.txt
statistics_for_metabolites_with_foldchange.txt	statistics_for_metabolites_with_foldchange.txt
statistics_for_metabolites_with_significance.txt	statistics_for_metabolites_with_significance.txt
statistics_for_metabolites_with_significance_and_foldchange.txt	statistics_for_metabolites_with_significance_and_foldchange.txt
VolcanoPLOT.pdf	VolcanoPLOT.pdf

Cannot Display File. No Corresponding viewer element.

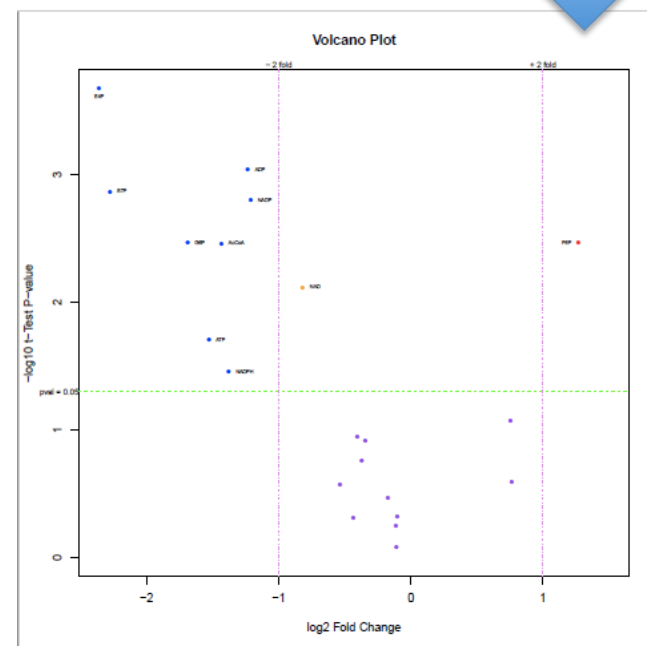
Open in System Editor

Click to see volcano visualization

Double click a row to download files

Launch

Process finished successfully





## INPUT

- Metabolite data

(.csv)

The gadget requires one input file; Shimadzu metabolome abundance data (e.g., test\_metabolome\_a.szf)

**Sample File:** Sample file to test is available under **ShimadzuGadgets\_SampleData > VolcanoPlotGenerator**

**NOTE:** Required package: R > 3.2.2 is required. "limma", "pcaMethods", "crmn", and "metabolomics" packages are required. The gadget automatically installs the packages in your computer, if the gadgets were not installed in your computer.

Volcano Plot Generator

Input Files

Output Files

Shimadzu Omics Data

test\_metabolome\_a.szf

Configuration

Shimadzu Omics Data					
compound name	CHEBI	Inchi	KEGG_COMPOUND	S2	
(Sample No)	*	*	*		0
G6P	CHEBI:4170	NBSCHQHZLSJFNQ-GASJEMHNSA-N	C00092		0.258
R5P	CHEBI:52742	KTVXPYOYAKDPRHY-SOOFDHINKSA-N	C00117		0.007
E4P	CHEBI:48153	NGHMDNPXVRFFGS-IUYQGCFVSA-N	C00279		0.046
S7P	CHEBI:15721	JDTUMPKOJBQPKX-GBNDHIKLSA-N	C05382		0.029
PYR	CHEBI:32816	LCTONWCANYUPL-UHFFFAOYSA-N	C00022		0.806
DHAP	CHEBI:16108	GNGACRATGGDKBX-UHFFFAOYSA-N	C00111		0.042
AMP	CHEBI:16027	UDMBCSSLTHINCD-KQYNXXCUSA-N	C00020		0.022
FBP	CHEBI:16905	XPYBSIWDXQFNMH-UYFOZJQFSA-N	C00354		5.428
3PG+2PG	CHEBI:17835		C00631		0.164
PEP	CHEBI:18021				0.029
6PG	CHEBI:48928				0.073
ADP	CHEBI:16761	XTWYTFMLZFPYCI-KQYNXXCUSA-N	C00008		0.012
ATP	CHEBI:15422	ZKHQWZAMYRWXGA-KQYNXXCUSA-N	C00002		0.399
AcCoA	CHEBI:15351	ZSLZBFCDGINBPY-ZSJPKINUSA-N	C00024		0.028
F6P	CHEBI:61553	BGWGXAPYGGQALX-VRPWFDXPXA-N	C00085		0.031
Xu5P			C00231		0.008
Ru5P	CHEBI:17363	FNZLKVNUWIIPSJ-UHNWVWZDZSA-N	C00199		0.002
NAD	CHEBI:15846	BAWFJGJZGIEFAR-NNYOXOHSSA-O	C00003		0.112
NADP	CHEBI:18009	XJLXINKUBYWONI-NNYOXOHSSA-O	C00006		0.042
NADH	CHEBI:16908	BOPGDPNILDQYTO-NNYOXOHSSA-N	C00004		0.006

File is displayed here

Rscript volcano\_plot.r test\_metabolome\_a.szf

Launch

Connected to Garuda

Double click a rows to load files



## [parameter settings]

1. Click “Configuration” on the left panel.
2. Select “Control” and “Target” samples for Volcano Plot Generator analysis.

In this example, “pfk1.b4.qgd, pfk1.b5.qgd, pfk1.b6.qgd” are selected as “Control” samples, while “zwf1.b7.qgd, zwf1.b8.qgd, zwf1.b9.qgd” are selected as “Target” samples.

3. Set threshold value of p-value and that of fold change for Volcano Plot Generator analysis.

In the example, 0.05 and 2 are selected as threshold values for p-value and fold-change, respectively.

4. Click the **bottom** to do Volcano Plot Generator analysis after data upload after data upload and parameter setting

The screenshot shows the Volcano Plot Generator web application. The interface includes a left sidebar with 'Input Files' and 'Output Files' tabs. The 'Input Files' tab is active, showing 'Shimadzu Omics Data' and 'test\_metabolome\_a.szf'. The 'Configuration' section is highlighted. A table lists various samples with checkboxes for 'Control' and 'Target' selection. Below the table, there are input fields for 'p-value' (0.05) and 'Fold Change' (2), both marked as mandatory. A 'Launch' button is at the bottom right. Four blue arrows with numbered circles (1-4) point to specific elements: 1 points to the 'Configuration' tab, 2 points to the 'Control' and 'Target' checkboxes, 3 points to the 'p-value' and 'Fold Change' input fields, and 4 points to the 'Launch' button.

Sample	Control*	Target*
compound name	<input type="checkbox"/>	<input type="checkbox"/>
ChEBI	<input type="checkbox"/>	<input type="checkbox"/>
Inchi	<input type="checkbox"/>	<input type="checkbox"/>
KEGG_COMPOUND	<input type="checkbox"/>	<input type="checkbox"/>
S288C:b1.qgd	<input type="checkbox"/>	<input type="checkbox"/>
S288C:b2.qgd	<input type="checkbox"/>	<input type="checkbox"/>
S288C:b3.qgd	<input type="checkbox"/>	<input type="checkbox"/>
pfk1:b4.qgd	<input checked="" type="checkbox"/>	<input type="checkbox"/>
pfk1:b5.qgd	<input checked="" type="checkbox"/>	<input type="checkbox"/>
pfk1:b6.qgd	<input checked="" type="checkbox"/>	<input type="checkbox"/>
zwf1:b7.qgd	<input type="checkbox"/>	<input checked="" type="checkbox"/>
zwf1:b8.qgd	<input type="checkbox"/>	<input checked="" type="checkbox"/>
zwf1:b9.qgd	<input type="checkbox"/>	<input checked="" type="checkbox"/>

p-value: 0.05  
Fold Change: 2  
\* Mandatory Fields

Rsript volcano\_plot.r test\_metabolome\_a.szf

Connected to Garuda

Launch

① ② ③ ④



## OUTPUT

- Statistics from Volcano Plot Generator analysis
- Metabolome abundance data from Volcano Plot Generator analysis.
- Volcano Plot Generator visualization (.szf)

## Statistics from Volcano Plot Generator analysis

Four result files for statistics will be generated by the volcano analysis gadget.

- “**statistics\_all.txt**” is statistics for all metabolites.
- “**statistics\_for\_metabolites\_with\_significance.txt**” is statistics for metabolites with p-value lower than user defined threshold value of p-value.
- “**statistics\_for\_metabolites\_with\_foldchange.txt**” is statistics for metabolites with foldchange greater than user defined threshold value.
- “**statistics\_for\_metabolites\_with\_significance\_and\_foldchange.txt**” is statistics for metabolites with p-value and foldchange that are lower and greater than user defined threshold values, respectively.

The screenshot shows the Volcano Plot Generator interface. The 'Output Files' tab is selected, displaying a list of generated files. A blue box highlights the first four files: **statistics\_all.txt**, **statistics\_for\_metabolites\_with\_foldchange.txt**, **statistics\_for\_metabolites\_with\_significance.txt**, and **statistics\_for\_metabolites\_with\_significance\_and\_foldchange.txt**. A blue arrow points from the text 'Double click a row to download files' to the first file in the list. To the right, the 'Results Panel' shows a table of metabolite data.

compound Name	"kegg id"	"t-statistic"	
G6P	C00092	-13.3306576525995	0.003
R5P	C00117	-0.817068173972164	0.486
E4P	C00279	-12.9043732505126	0.000
S7P	C05382	-16.1711972751795	0.001
PYR	C00022	-1.13428079417541	0.342
DHAP		123294734	0.084
AMP		2256841475	0.469
FBP		1945213	0.255
3PG+2PG	C00631	-2.42061092514349	0.121
PEP	C00074	-2.56191032522519	0.113
3PG	C00345	-1.85185763881223	0.172
ADP	C00008	-11.0953007490424	0.000
ATP	C00002	-5.64721273310225	0.019
AcCoA	C00024	-6.21822952748817	0.003
6P	C00085	7.53279330473999	0.003
u5P	C00231	-0.253616731056512	0.818
u5P	C00199	-1.31353993489225	0.265
NAD	C00003	-5.11842762503984	0.007
NADP	C00006	-7.63118125647089	0.001
NADH	C00004	-0.692470874999738	0.560
NADPH	C00005	-3.46359240742034	0.035

At the bottom, a text box contains the command: `Rscript volcano_plot.r test_metabolome_a.szf` and a 'Launch' button. A status message at the bottom reads: 'Process finished successfully'.

Double click a row to download files



## OUTPUT

- Statistics from Volcano Plot Generator analysis
- Metabolome abundance data from Volcano Plot Generator analysis.**
- Volcano Plot Generator visualization (.szf)

## Metabolome abundance data from Volcano Plot Generator analysis.

Three files for metabolome abundance will be generated by the volcano analysis gadget.

- “**abundance\_for\_metabolites\_with\_significance.szf**” is abundance for metabolites with p-value lower than user defined threshold value of p-value.
- “**abundance\_for\_metabolites\_with\_foldchange.szf**” is abundance for metabolites with fold change greater than user defined threshold value.
- “**abundance\_for\_metabolites\_with\_significance\_and\_foldchange.szf**” is abundance for metabolites with p-value and fold change that are lower and greater than user defined threshold values, respectively.

Volcano Plot Generator

Input Files Output Files

abundance\_for\_metabolites\_with\_foldchange.szf  
abundance\_for\_metabolites\_with\_foldchange.szf  
abundance\_for\_metabolites\_with\_significance.szf  
abundance\_for\_metabolites\_with\_significance\_and\_foldchange.szf  
log.txt  
statistics\_all.txt  
statistics\_for\_metabolites\_with\_foldchange.txt  
statistics\_for\_metabolites\_with\_significance.txt  
statistics\_for\_metabolites\_with\_significance\_and\_foldchange.txt  
VolcanoPLOT.pdf  
VolcanoPLOT.pdf

"compound names"	"ChEBI"	"Inchi"
1	*	*
E4P	CHEBI: 48153	NGHMDNPXVRFSG-IUYQGCY
ADP	CHEBI: 16761	XTWYTFMLZFPYCI-KQYNXXCU
S7P	CHEBI: 15721	JDTUMPKOJBQPKX-GBNDHKL
NADP	CHEBI: 18009	XJLXINKUBYWONI-NINYOXOHS
F6P	CHEBI: 61553	BGWGXPPYGGQALX-VRPWDFP
G6P		INQ-GASJEMH
AcCoA		PY-ZSJPKNUS
ATP	CHEBI: 15722	LNPLQVWZAMITKWXGA-KQYNXX
NADPH	CHEBI: 16474	ACFIXIJJZMPPPO-NINYOXOHS

Results Panel

Rscript volcano\_plot.r test\_metabolome\_a.szf

Launch

Process finished successfully

Double click a row to download files



## OUTPUT

- Statistics from Volcano Plot Generator analysis
- Metabolome abundance data from Volcano Plot Generator analysis.
- Volcano Plot Generator visualization (.szf)**

## Volcano Plot Generator visualization

- Click on the right panel to display volcano visualization.
- Double click the row "VolcanoPLOT.pdf" to download files.

Volcano Plot Generator

Input Files Output Files

Discover File Data ?

abundance_for_metabolites_with_foldchange.szf	abundance_for_metabolites_with_foldchange.szf
abundance_for_metabolites_with_significance.szf	abundance_for_metabolites_with_significance.szf
abundance_for_metabolites_with_significance_and_foldchange.szf	abundance_for_metabolites_with_significance_and_foldchange.szf
log.txt	log.txt
statistics_all.txt	statistics_all.txt
statistics_for_metabolites_with_foldchange.txt	statistics_for_metabolites_with_foldchange.txt
statistics_for_metabolites_with_significance.txt	statistics_for_metabolites_with_significance.txt
statistics_for_metabolites_with_significance_and_foldchange.txt	statistics_for_metabolites_with_significance_and_foldchange.txt
VolcanoPLOT.pdf	VolcanoPLOT.pdf

Cannot Display File. No Corresponding viewer element.

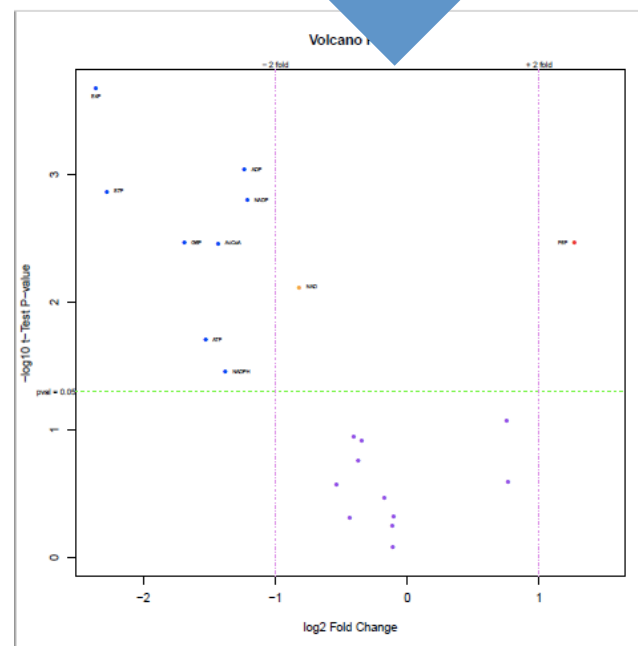
Open in System Editor

Click to see volcano visualization

Double click a row to download files

Process finished successfully

Launch







# Blank GML Generator

This Gadget generates blank .gml file from a list of metabolites and that of associations between the metabolites. A blank .gml file from this gadget will be used as input for “Multiomics Data Mapper” gadget.

## INPUT

- List of Metabolites
- the association between these metabolites



(.csv)

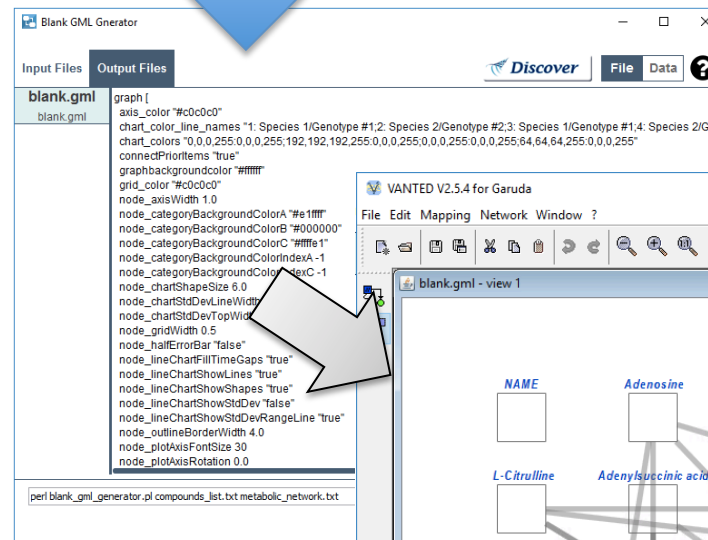
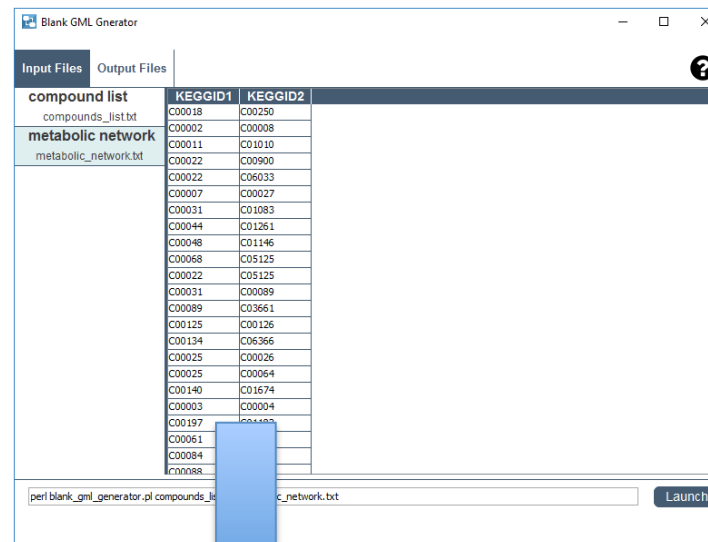


- Generate a blank .gml file for “VANTED”

## OUTPUT

- A blank .gml file  
→ use as an input for Multiomics Data Mapper gadget

(.gml)





# Blank GML Generator

## INPUT

- List of Metabolites



- the association between these metabolites

(.csv)

The gadget requires two input files;

- (1) a table for metabolites

(e.g., compounds\_list.txt)

- (2) network composed of links between two metabolites (e.g., metabolic\_network.txt)

1. Double click a row to load files
2. Click the “Launch” button to make blank .gml file after data upload

### Sample File:

Sample file to test is available under  
**ShimadzuGadgets\_SampleData>**  
**BlankGMLGenerator**

KEGGID1	KEGGID2
C00018	C00250
C00002	C00008
C00011	C01010
C00022	C00900
C00022	C06033
C00007	C00027
C00031	C01083
C00044	C01261
C00048	C01146
C00068	C05125
C00022	C05125
C00031	C00089
C00089	C03661
C00125	C00126
C00134	C06366
C00025	C00026
C00025	C00064
C00140	C01674
C00003	C00004
C00197	C01182
C00061	C01847
C00084	C18091
C00088	C18091



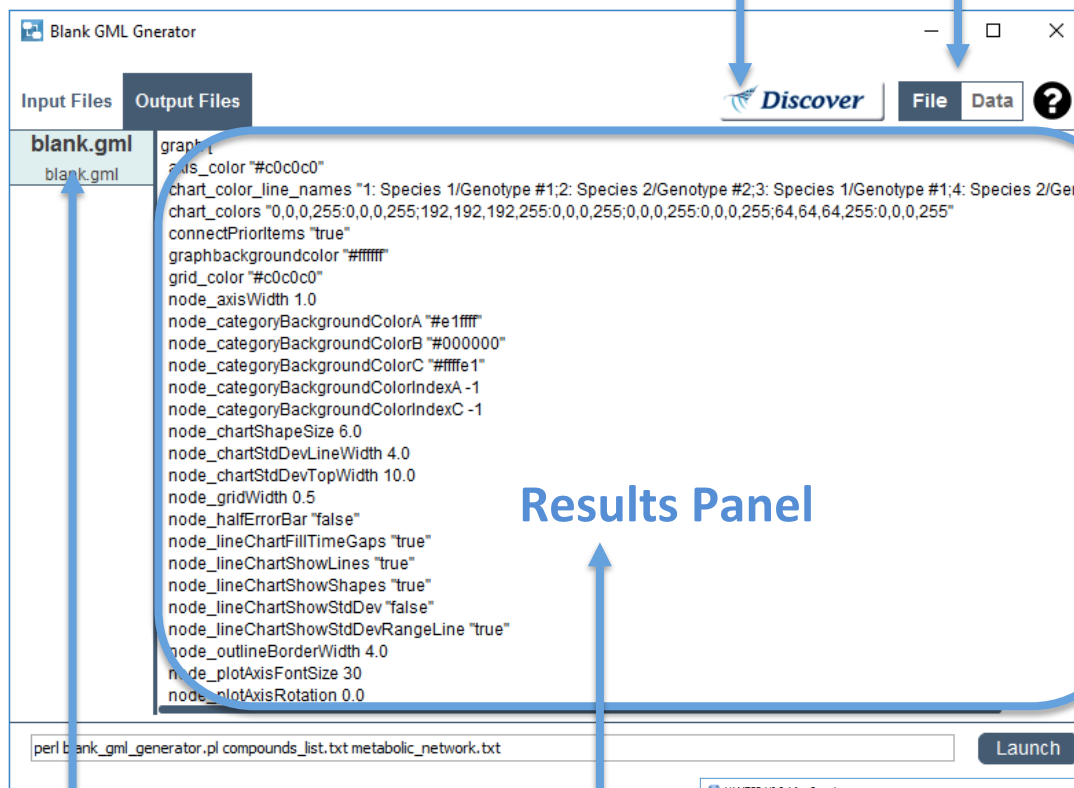
# Blank GML Generator

## OUTPUT

- A blank .gml file  
→ use as an input for Multiomics Data Mapper gadget

(.gml)

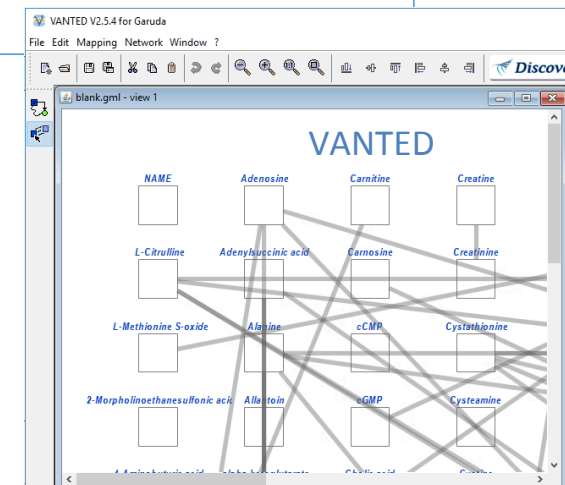
- Select whether you want to send the entire **File** or some **Data** to other gadgets
- Click **Discover** to send data to other gadgets



Results Panel

Double click a rows to download files

Resultant merged gml is shown in the result panel





# Multiomics Data Mapper

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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.

## INPUT

- Merged .szf data output from Shimadzu MSdata Import



(.szf)

- GML file for VANTED

(.gml)



- Merge Shimadzu multi-omics data with GML file for VANTED

## OUTPUT

- Send data to VANTED

(.gml)

Multiomics Data Mapper

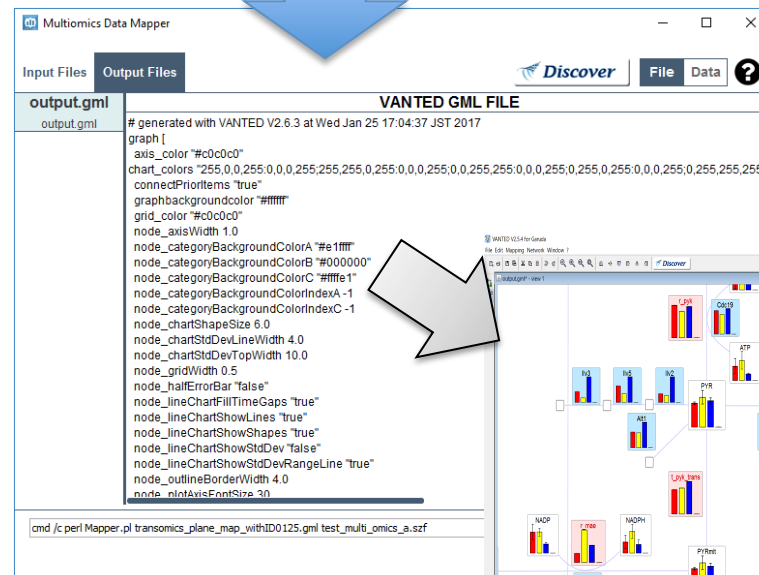
Input Files: transomics\_plane\_map\_withID0125.gml, Shimadzu Multi-omics Data test\_multi\_omics\_a.szf

Output Files:

(Sample No)	compound name	ChEBI	Inchi	KEGG COM
G6P		CHEBI:4170	NBSCHQZLSJFNQ-GASJEMHNSA-N	C00092
R5P		CHEBI:52742	KTVPOYAKDPHY-SOOFDHNSA-N	C00117
E4P		CHEBI:48153	NGHMDNPXVRFPGS-IUYQCFVSA-N	C00279
S7P		CHEBI:15721	JDTUMPKOJBQPKX-GBNDHLSA-N	C05382
PYR		CHEBI:32816	LCTONWCANYPML-UHFFFAOYSA-N	C00022
DHAP		CHEBI:16108	GNAGCRATGDKBX-UHFFFAOYSA-N	C00111
AMP		CHEBI:16027	UDMBCCSLTHNCD-KQYNOCUSA-N	C00020
FBP		CHEBI:16905	XPYBSTWDXQFMH-UFOZJQFSA-N	C00354
3PG+2PG		CHEBI:17835		C00631
PEP		CHEBI:18021	DTBNBXWJWCWCK-UHFFFAOYSA-M	C00074
6PG		CHEBI:48928	BIRSGZKFKLSJQ-SQOUGZOYSA-N	C00345
ADP		CHEBI:16761	XTWYTFMLZFPYCI-KQYNOCUSA-N	C00008
ATP		CHEBI:15422	ZKHQWZAMYRVXGA-KQYNOCUSA-N	C00002
AcCoA		CHEBI:15351	ZSLZBFDCINBPY-ZSJKINUSA-N	C00024
F6P		CHEBI:61553	BGVGXAPYQALX-VRPWFDPKSA-N	C00085
Xu5P				C00231
Ru5P		CHEBI:17363	FNZLVNLUWIPJSJ-UHNWVZDZSA-N	C00199
NAD		CHEBI:15846	BAWFXGJZGIEFAR-NNYOXHSSA-O	C00003
NADP		CHEBI:18009	XJLXINKUBYWONI-NNYOXHSSA-O	C00006
NADH		CHEBI:16908	BOPGDPNLDQYTO-NNYOXHSSA-N	C00004
NADPH		CHEBI:16474	ACFXJLJLZMPPG-NNYOXHSSA-N	C00005

cmd /c perl Mapper.pl transomics\_plane\_map\_withID0125.gml test\_multi\_omics\_a.szf

Launch





# Multiomics Data Mapper

## INPUT

- Merged .szf data output from Shimadzu MSdata Import



(.szf)

- .gml file for VANTED

(.gml)

The gadget requires two input files;

- gml file** for blank metabolic pathway map (e.g., transomics\_plane\_map\_withID0125.gml)
- Shimadzu multi-omics dataset** (e.g., test\_multi\_omics\_a.szf)

**Sample File:** Sample file to test is available under ShimadzuGadgets\_SampleData> MultiomicsDataMapper

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

Multiomics Data Mapper

Input Files | Output Files

**Pathway GML File**  
transomics\_plane\_map\_withID0125.gml

**Shimadzu Multi-omics Data**  
test\_multi\_omics\_a.szf

Double click a rows to load files

compound name	CHEBI	Inchi	KEGG_COM
(Sample No)	*	*	*
G6P	CHEBI:4170	NBSCHQHLSJFNQ-GASJEMHNSA-N	C00092
R5P	CHEBI:52742	KTVPXOYAKDPRHY-SOOFDHINKSA-N	C00117
E4P	CHEBI:48153	NGHMDNPXVRRFFGS-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	CHEBI:16027	UDMBCSSLTHHNCDC-KQYNXXCUSA-N	C00020
FBP	CHEBI:16905	XPYBSIWDXQFNMH-UYFOZJQFSA-N	C00354
3PG+2PG			C00631
PEP			C00074
6PG			C00345
ADP	CHEBI:16761	XTWYTFMLZFPYCI-KQYNXXCUSA-N	C00008
ATP	CHEBI:15422	ZKHQWZAMYRWXGA-KQYNXXCUSA-N	C00002
AcCoA	CHEBI:15351	ZSLZBFCDCINBPY-ZSJPKINUSA-N	C00024
F6P	CHEBI:61553	BGWXPAPYQGALX-VRPWFDPXSA-N	C00085
Xu5P			C00231
Ru5P	CHEBI:17363	FNZLKVNUWIIPSJ-UHNVWZDZSA-N	C00199
NAD	CHEBI:15846	BAWFJGJGIEFAR-NINYOXOHSSA-O	C00003
NADP	CHEBI:18009	XJLXINKUBYWONI-NINYOXOHSSA-O	C00006
NADH	CHEBI:16908	BOPGDPNILDQYTO-NINYOXOHSSA-N	C00004
NADPH	CHEBI:16474	ACFIXJJDZMPPPO-NINYOXOHSSA-N	C00005

File is displayed here

cmd /c perl Mapper.pl transomics\_plane\_map\_withID0125.gml test\_multi\_omics\_a.szf

Launch

Click the bottom to map multiOmics data on metabolic network (.gml file) after data upload



## OUTPUT

- Send data to VANTED

(.gml)

- Select whether you want to send the entire **File** or some **Data** to other gadgets
- Click **Discover** to send data to other gadgets

The screenshot shows the Multiomics Data Mapper application window. At the top, there are tabs for 'Input Files' and 'Output Files'. The 'Output Files' tab is active, showing a list of output files including 'output.gml'. To the right of the tabs are buttons for 'Discover', 'File', 'Data', and a help icon. A blue arrow labeled '2' points to the 'Discover' button, and a blue arrow labeled '1' points to the 'File' button. Below the tabs, the 'VANTED GML FILE' section displays a GML file content. A blue rounded rectangle highlights this section, with a blue arrow pointing to it from the text 'Results Panel'. At the bottom of the window, there is a command line input field containing the command: 'cmd /c perl Mapper.pl transomics\_plane\_map\_withID0125.gml test\_multi\_omics\_a.szf'. A blue arrow points from the text 'Resultant merged gml is shown in the result panel' to this command line. A 'Launch' button is located to the right of the command line.

```
# 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;0,0,0,255;255,255,0,255;0,0,0,255;0,0,255,255;0,0,0,255;0,255,0,255;0,0,0,255;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 "t"
  node_lineChartShowLines "tru"
  node_lineChartShowShapes "true"
  node_lineChartShowStdDev "false"
  node_lineChartShowStdDevRangeLine "true"
  node_outlineBorderWidth 4.0
  node_outlineFontStyle 0.0
```

cmd /c perl Mapper.pl transomics\_plane\_map\_withID0125.gml test\_multi\_omics\_a.szf

Resultant merged gml is shown in the result panel

# Garuda Recipes

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## Garuda Recipes – Analytics Pipelines

- This section outlines the **different analytic pipelines (called Garuda Recipes)** which can be constructed with the gadgets outlined in this document and connecting with available community gadgets.
- Specifically, the recipes elucidated in the following slides are built by connecting the multi-omics gadgets with the following **community gadgets\***
  - iPATH2
  - VANTED
- **All samples** for the gadgets and recipes are in **the Samples folder**

## Community Gadgets used with Shimadzu Multiomics Analysis gadgets

There are 2 community gadgets used for Shimadzu multi-omics data analysis pipeline.



### VANTED

This gadget uses a .gml file output from “Multiomics Data Mapper” gadget to visualize metabolome abundance data on metabolome pathway map through software VANTED.



### iPATH2

This gadget maps and visualizes KEGG ids on KEGG pathways maps

**NOTE:** \* Please note that **the community gadgets** are developed and made available by the Garuda Alliance members and not included in the scope of the collaboration with Shimadzu and Osaka University





This gadget uses a .gml file output from “**Multionics Data Mapper**” gadget to visualize metabolome abundance data on metabolome pathway map through software VANTED.

## INPUT

- .gml file from “Multionics Data Mapper” gadget

(.GML)

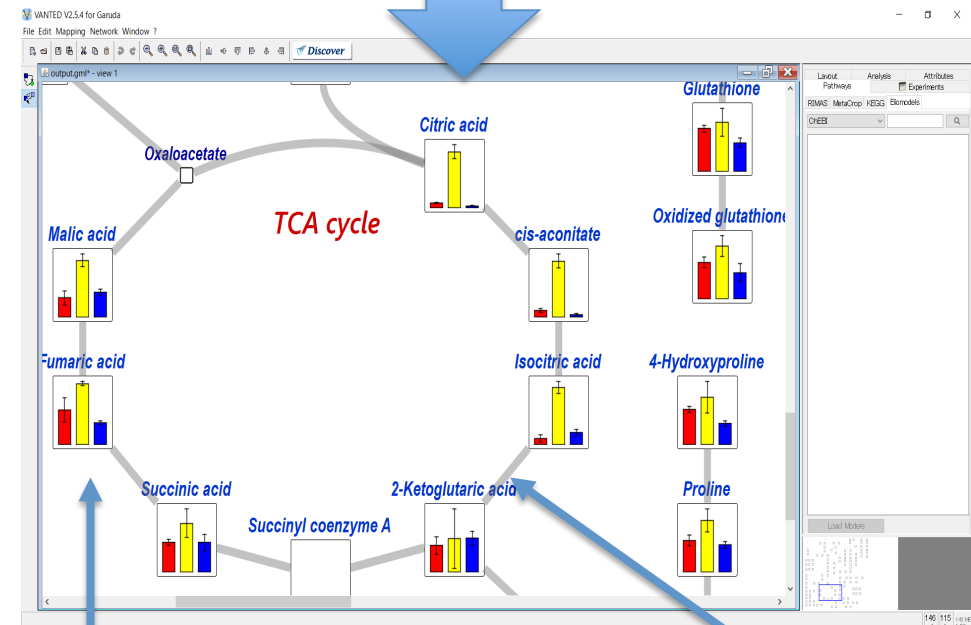
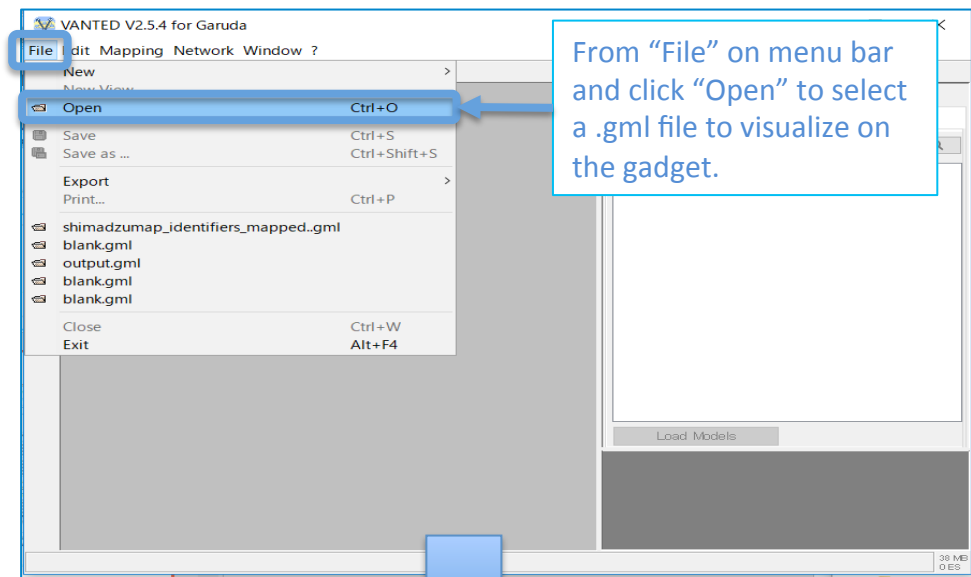


- Visualize multiomics data over VANTED pathway map.

## OUTPUT

- Image file

(.png)



This gadget maps and visualizes KEGG ids on KEGG pathway maps

## INPUT

- KEGG IDs

(.szf / .txt)

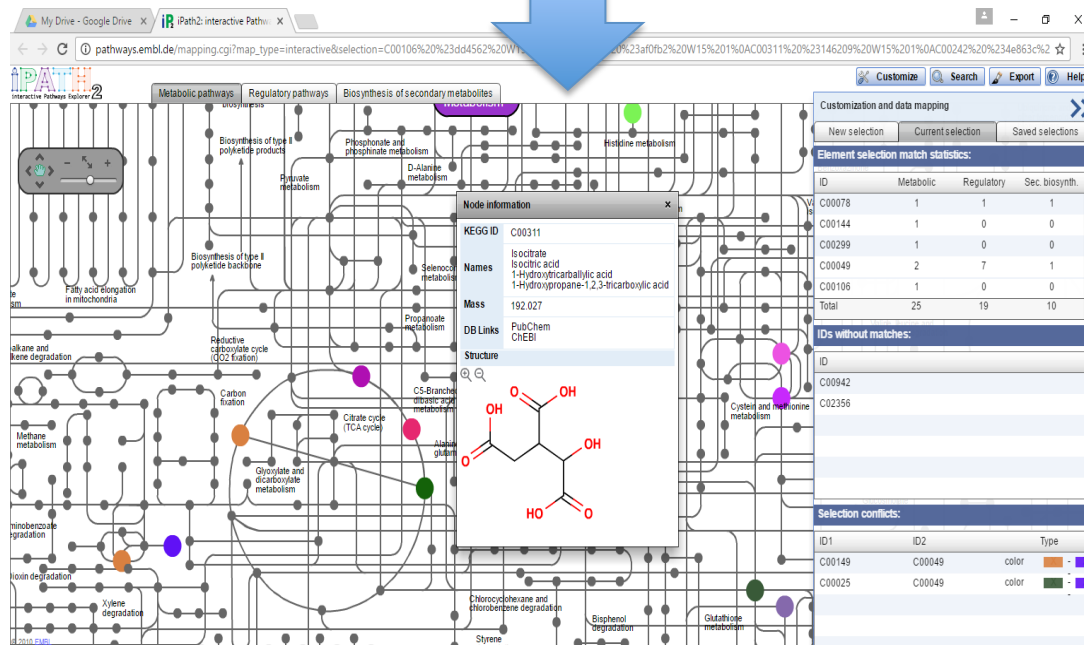
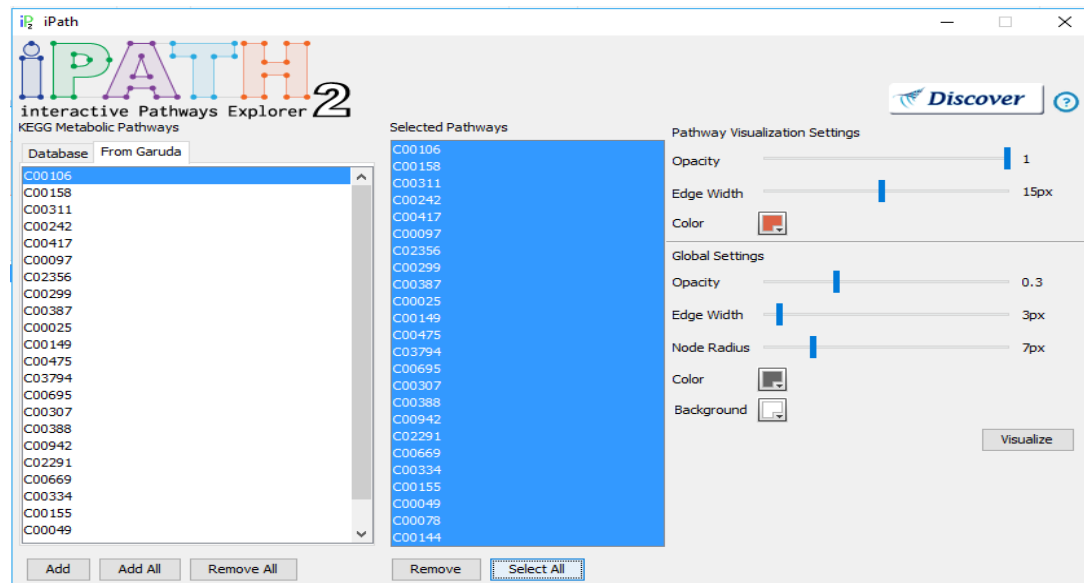


- Visualize KEGG ids on KEGG pathway maps

## OUTPUT

- Image file

(.png)

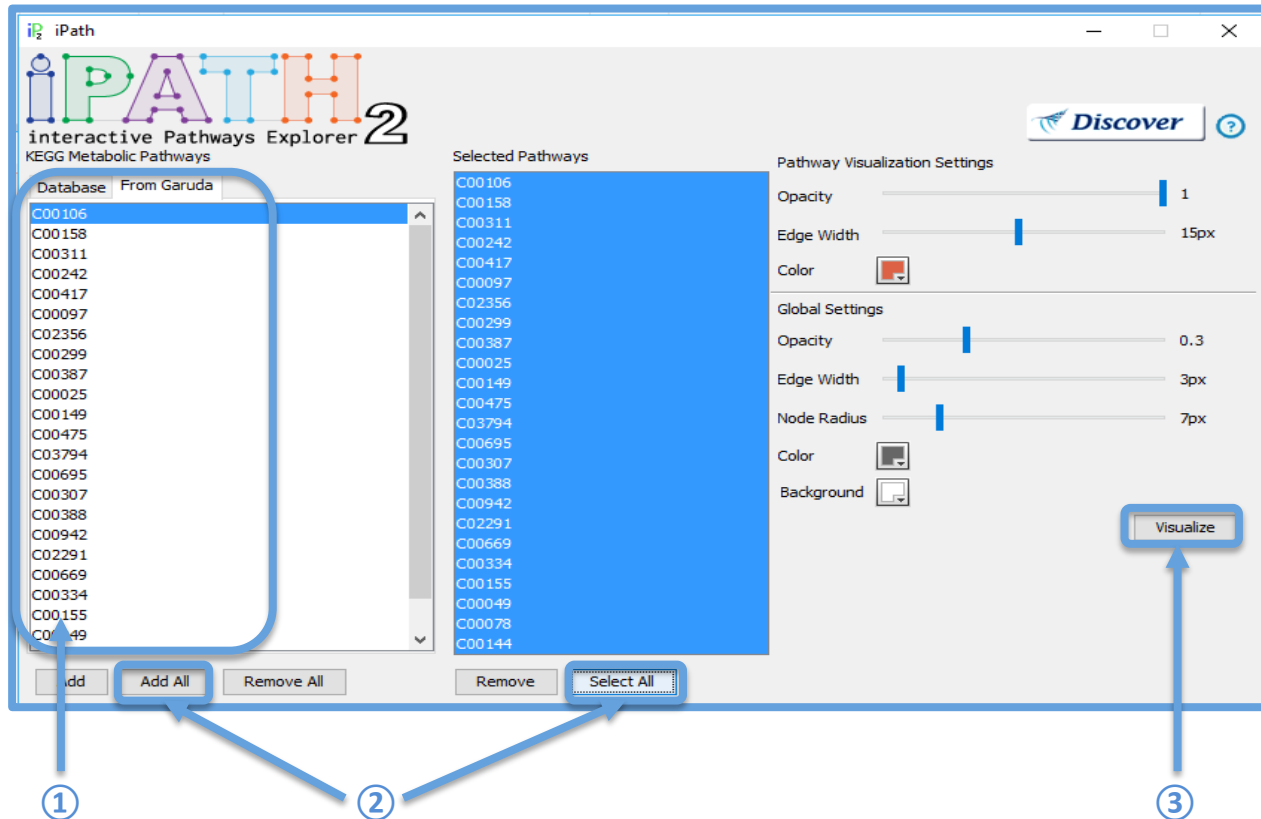


This gadget maps and visualizes KEGG ids on KEGG pathway maps



[parameter settings]

1. List of metabolites uploaded from an other gadget.
2. Click “Add All” and “Select All” to select all metabolites from other gadgets to visualize on KEGG map.
3. Click to **launch** iPath2 Visualizer.



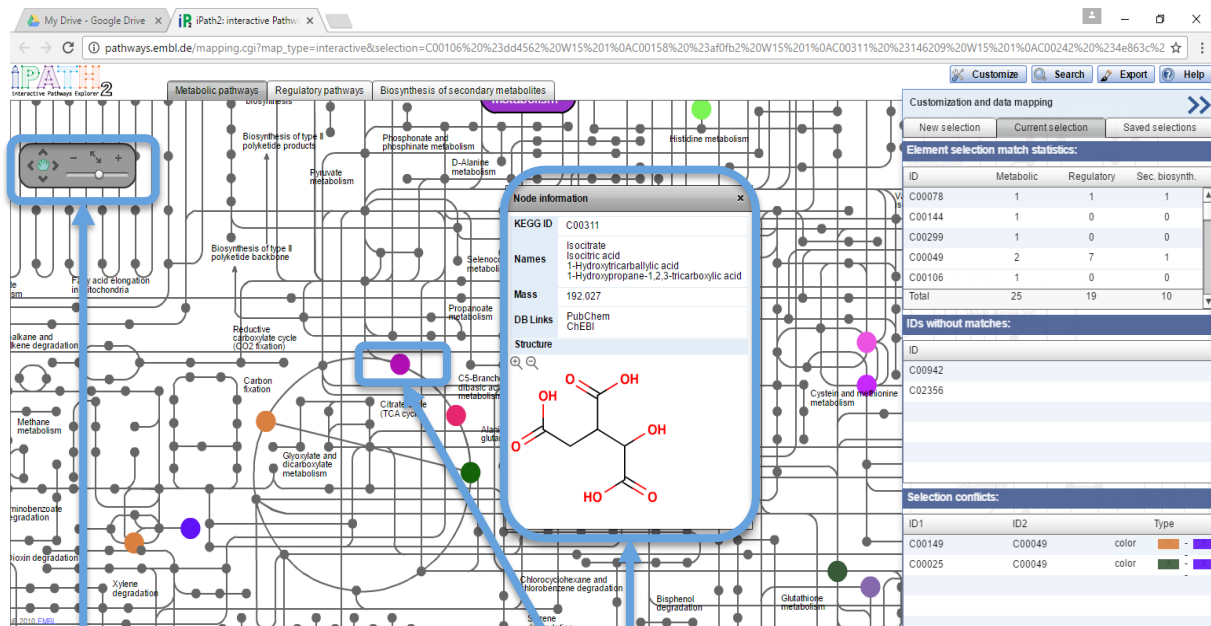
The screenshot shows the iPath2 Interactive Pathways Explorer interface. The interface includes a 'Database' tab with a list of metabolites (C00106, C00158, C00311, C00242, C00417, C00097, C02356, C00299, C00387, C00025, C00149, C00475, C03794, C00695, C00307, C00388, C00942, C02291, C00669, C00334, C00155, C00149). Below the list are buttons: 'Add', 'Add All', 'Remove All', 'Remove', and 'Select All'. The 'Add All' and 'Select All' buttons are highlighted with a blue box and labeled with a circled '2'. A blue arrow labeled '1' points to the 'Add' button. A blue arrow labeled '3' points to the 'Visualize' button in the bottom right corner. The interface also features a 'Selected Pathways' list on the right, 'Pathway Visualization Settings' (Opacity, Edge Width, Color), and 'Global Settings' (Opacity, Edge Width, Node Radius, Color, Background). A 'Discover' button is located in the top right corner.

This gadget maps and visualizes KEGG ids on KEGG pathway maps



[Visualize]

- Click to **zoom up/down** the map and to **explore** the map.
- Selected metabolites** are enlarged and colored on the map. Click to see details about the metabolites.

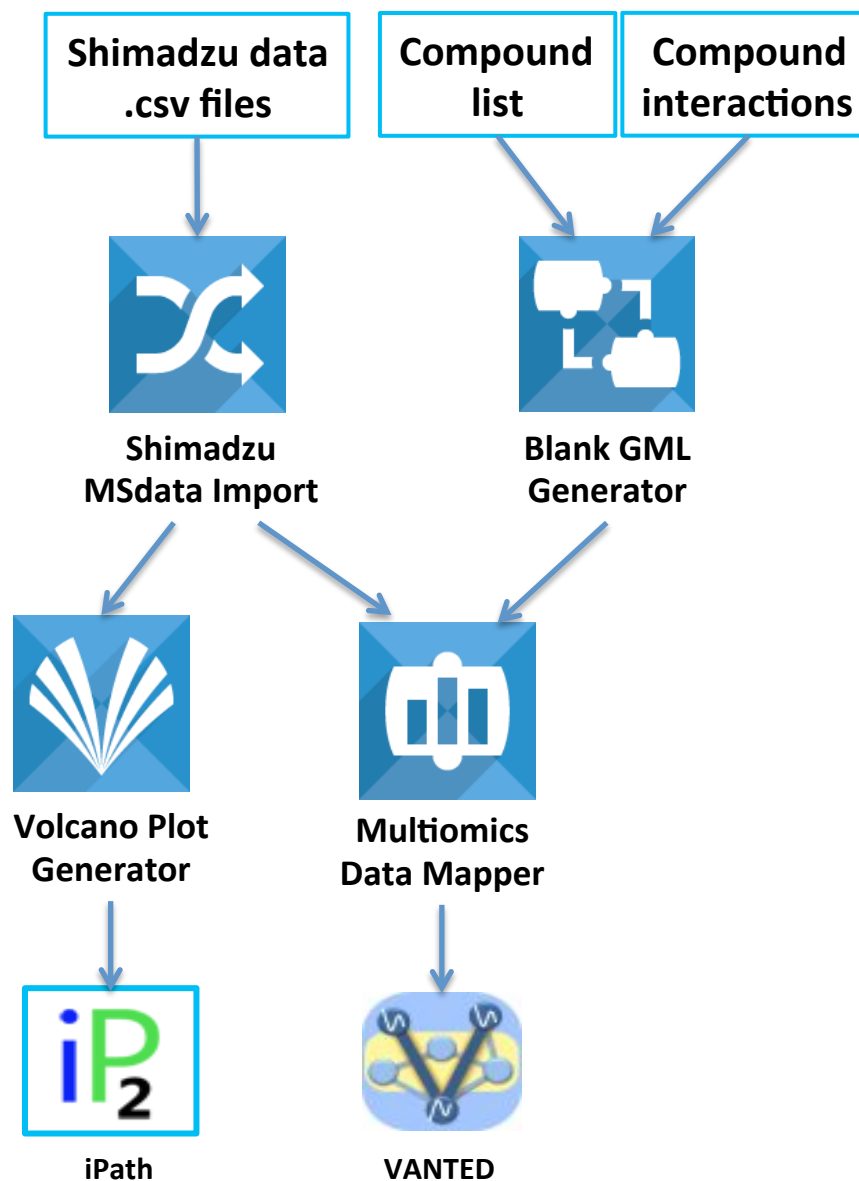


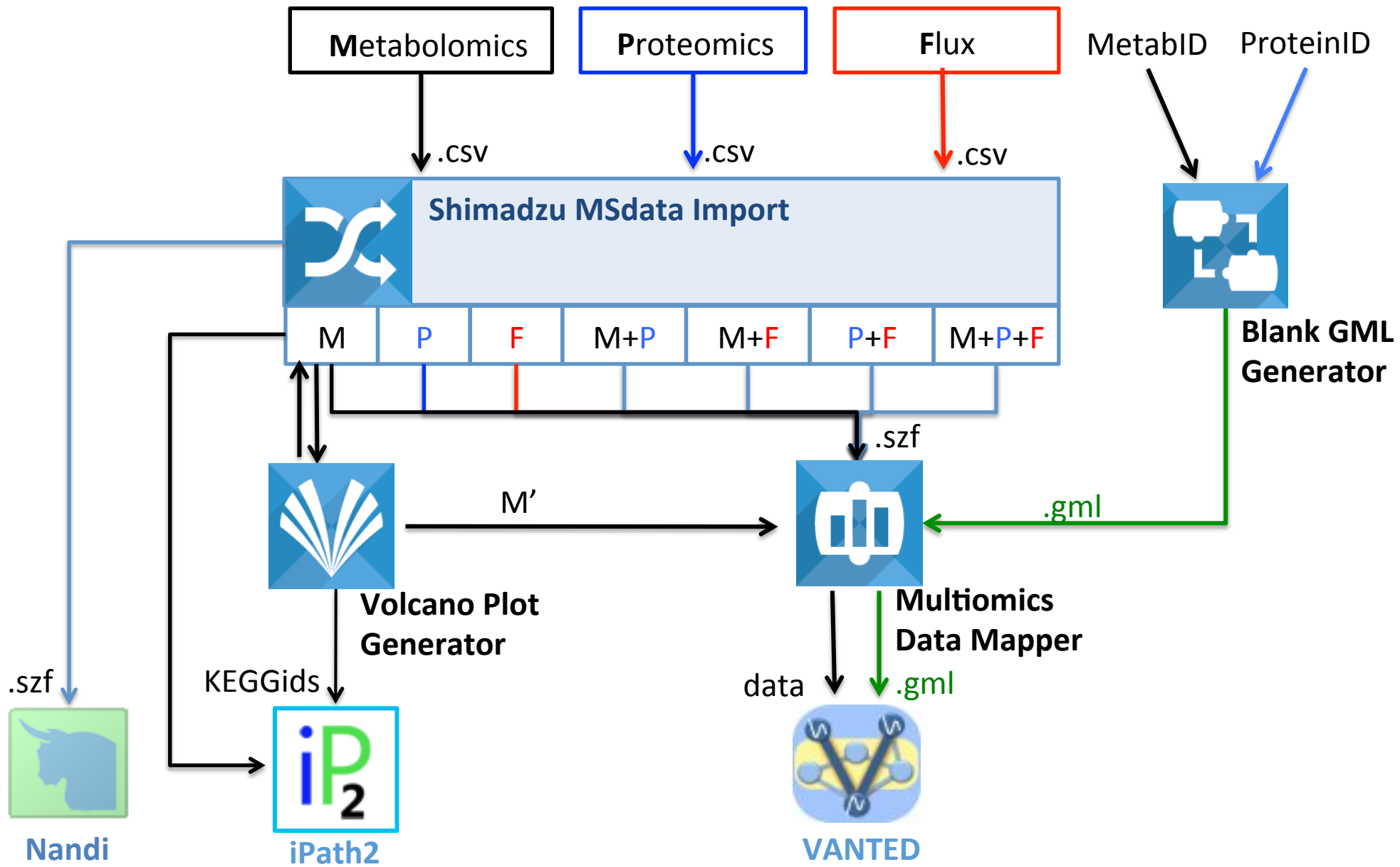
Click to zoom up/down the map and to explore the map.

Selected metabolites are enlarged and colored on the map. Click to see details about the metabolites.

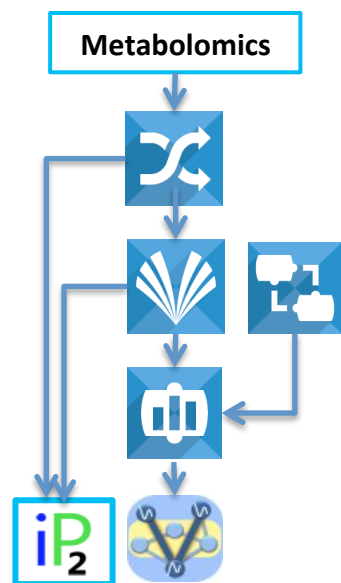
# Multionics Data Analysis Recipes Examples

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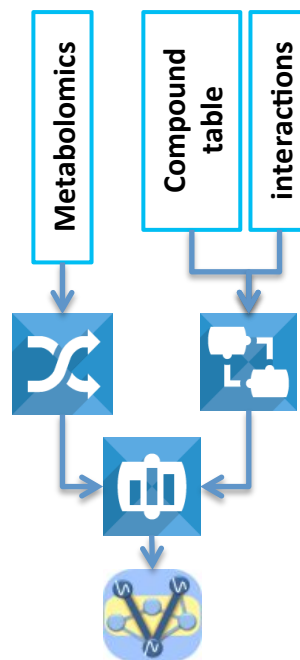




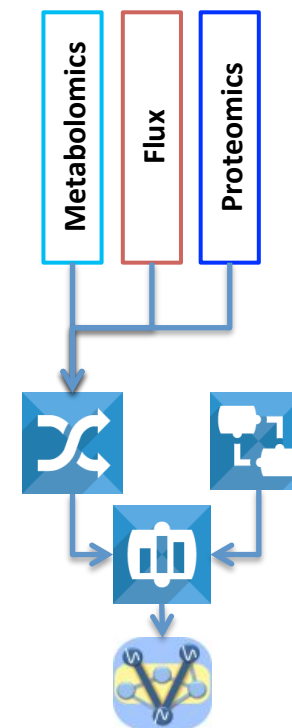
## Recipe #1 : Visualize Metabolite Data to Metabolomic Pathway



## Recipe #2 : Visualize Metabolite Data to Metabolomic Pathway on VANTED



## Recipe #3 : Visualize Multiomics Data to VANTED pathway



# Recipe #1 : Visualize Metabolite Data to Metabolomic Pathway

The recipe conducts **Volcano Plot Generator analysis** to identify significant metabolites.

Then abundance of the significant metabolites are mapped on the metabolic network through “iPath” or “Vanted”

## Input

- Metabolite quant data

(from LabSolutions Insight)

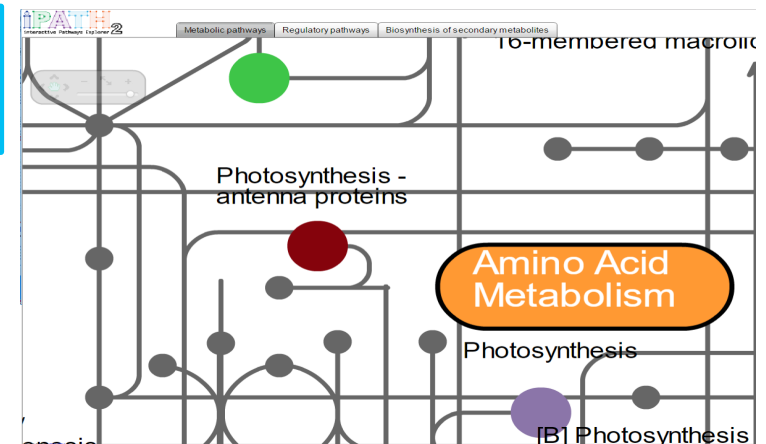
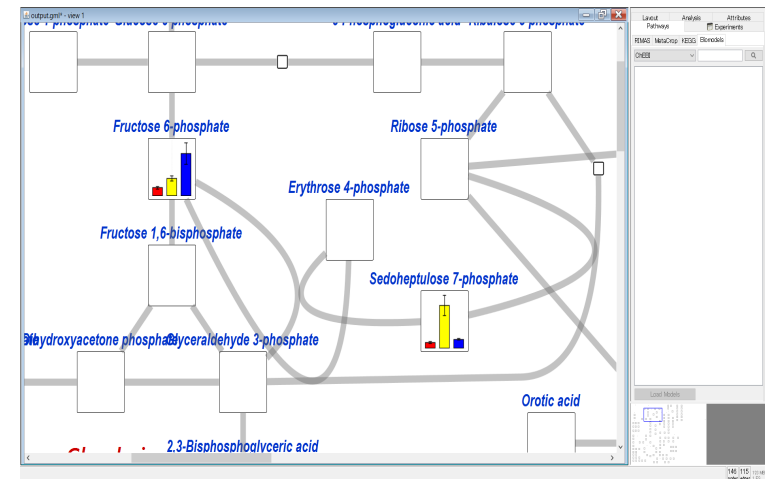
<http://www.shimadzu.com/an/data-net/labsolutions/insight/index.html>



## Gadgets for Cooking Data

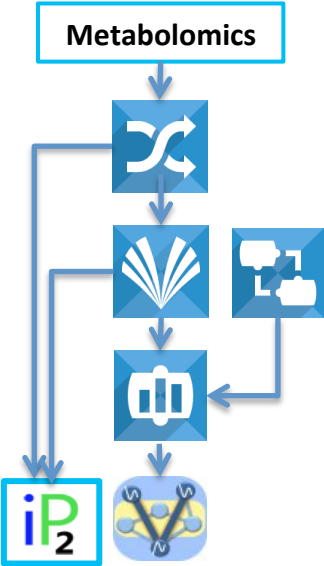
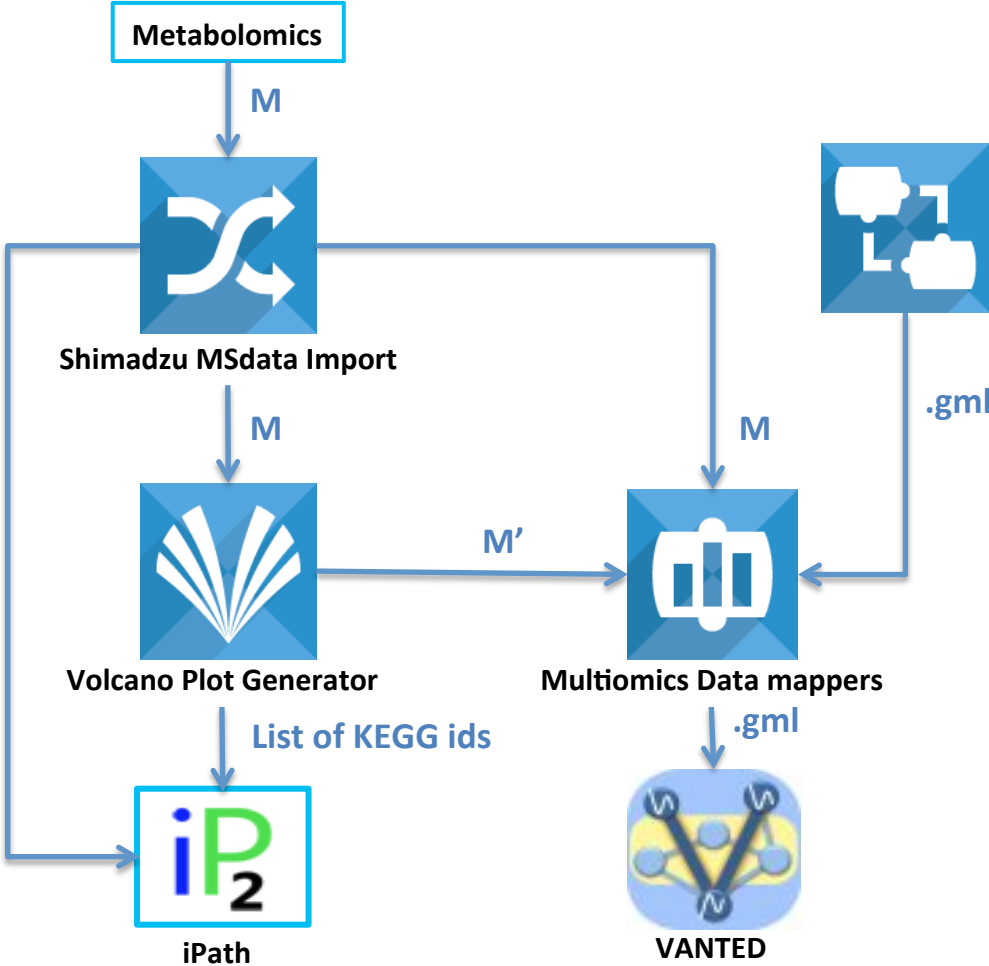


## OUTPUT





The recipe conducts **Volcano Plot Generator analysis** to identify significant metabolites. Then abundance of the significant metabolites are **mapped on the metabolic network** through “iPath”



# Recipe #1 : Visualize Metabolite Data to Metabolomic Pathway

## Metabolomics

### STEP 1. Format the Shimadzu metabolome abundance data for downstream analysis gadgets

- From the Garuda dashboard, select and double-click the **“Shimadzu MSdata Import”** gadget to launch the gadget.
- Click **“File”** and **“Open Metabolite Quant File”** to select and import the sample metabolome abundance data (**“Sample\_multi\_omics\_metabolome\_data.csv”** in **ShimadzuGadgets\_SampleData>ShimadzuMSdataImport**).
- Click **“Discover”** to list up gadget for downstream analysis. Select and double click **Gadget** (in this recipe, **“Volcano Plot Generator”**). You can upload the formatted data on the selected gadget.

Shimadzu MS data Import

②

Add Protein quant File(.csv)  
Add Metabolite quant File(.csv)  
Add Flux quant File(.csv)  
Exit

Selected Rows ☐ Merge by Sample No.  
☐ Merge by Sample  
☐ Avg. of timecourse

Output Style  
☒ Table  
☐ List

Load Initial Data Clear Data

select	Name	CHEBI	Inchi	kegg	S288CS288C_1_m	S288CS288C_2_m	S288CS288C_3_m	pkf.Idetapfk.1.1_m	pkf.Id
(Sample Name)	(Sample Name)	*	*	*	S288C	S288C	S288C	0	0
(Sample ID)	(Sample ID)	*	*	*	0	0	0	0	0
(time course)	(time course)	*	*	*	0	0	0	0	0
(replicate)	(replicate)	*	*	*	0	0	0	0	0
1	G6P	4170	NBSCHOHZLSJ...	C00092	0.255	0.315	0.288	0.819	0.721
2	R5P	52742	KTVPYOYAKDP...	C00117	0.007	0.01	0.008	0.022	0.017
3	E4P	48153	NGHMDNPXVRF...	C00279	0.046	0.053	0.047	0.263	0.263
4	S7P	15721	JOTUMPKOJBQ...	C05382	0.029	0.038	0.032	0.234	0.24
5	PYR	32816	LCTONWCANYU...	C00022	0.806	0.825	0.763	1.092	0.812
6	DHAP	16108	GNACRATGGD...	C00111	0.042	0.081	0.068	0.054	0.041
7	AMP	16027	UDMBCSSLTHL...	C00020	0.023	0.017	0.01	0.015	0.015
8	FBP	16905	XPYBSMDXQFN...	C00354	5.428	5.214	4.981	1.916	1.755
9	3PG*2PG	17835	C00197	C00631	0.164	0.225	0.17	0.201	0.206
10	PEP	18021	DTENBXWJWCW...	C00074	0.029	0.038	0.026	0.043	0.046
11	6PG	48928	BIRSQZKFJOLS...	C00345	0.073	0.075	0.073	0.092	0.078
12	ADP	16761	XTWYTFMLZFPY...	C00008	0.012	0.054	0.034	0.053	0.044
13	ATP	15422	ZKHQWZAMYRW...	C00002	0.399	0.633	0.313	0.609	0.434
14	AcCoA	15351	ZSLZBFDCINB...	C00024	0.028	0.045	0.024	0.043	0.031
15	F6P	61553	BGW3XPAPYGO...	C00085	0.031	0.025	0.03	0.061	0.058
16	Xu5P			C00231	0.008	0.013	0.012	0.023	0.02
17	Ru5P	17363	FNZLKVNUNWPS...	C00199	0.002	0.005	0.005	0.012	0.008
18	NAD	15846	BAWFJQJZGIEF...	C00003	0.112	0.169	0.112	0.144	0.162
19	MAN6	10000	V...	C00006	0.043	0.06	0.057	0.047	0.04

Shimadzu MS data Import

File(E) Data(D) Filter

View  
☐ Show : Dose Row  
☐ Show : 2 Rows  
☐ Hide ID Columns

☐ Normalize by Selected Rows  
☐ Merge by Sample No.  
☒ Merge by Sample  
☒ Avg. of timecourse

Output Style  
☒ Table  
☐ List

Select All Deselect All Deselect Columns Load Initial Data Clear Data

③ Discover

Nandi File Gateway  
Shimadzu MSdata Import  
Volcano Plot Generator

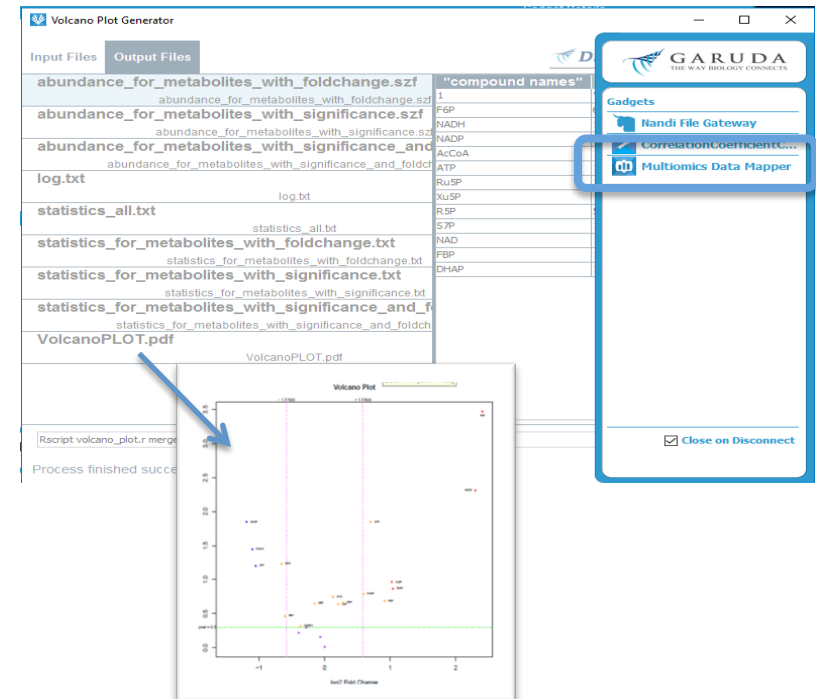
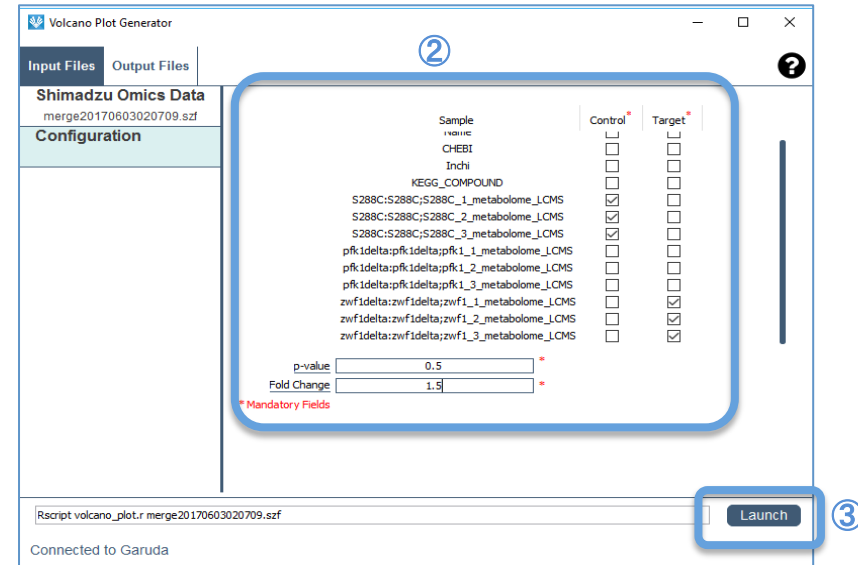
select	Name	eptide	Prefered name	UniProt	map1	map2
(Sample Name)	(Sample Name)	*	*	*	*	*
(Sample ID)	(Sample ID)	*	*	*	*	*
(time course)	(time course)	*	*	*	*	*
(replicate)	(replicate)	*	*	*	*	*
1	G6P					
2	R5P					
3	E4P					
4	S7P					
5	PYR					
6	DHAP					
7	AMP					
8	FBP					
9	3PG*2PG					
10	PEP					
11	6PG					
12	ADP					
13	ATP					
14	AcCoA					

# Recipe #1 : Visualize Metabolite Data to Metabolomic Pathway

## Metabolomics

### STEP 2. Volcano Plot Generator analysis for Shimadzu metabolome abundance

- From “**Shimadzu MSdata Import**”, select and double click “**Volcano Plot Generator**”. Garuda will launch the gadget and send the formatted data to the gadget.
- Set **parameters** (e.g., p-value and fold-change threshold as well as control and target samples). Please see help of “Volcano Plot Generator” gadget for details of the parameters.  
(In this example, “S288C.b1.qgd, S288C.b2.qgd, S288C.b4.qgd” are “**Control**” samples, while “zwf1.b7.qgd, zwf1.b8.qgd, zwf1.b9.qgd” are “**Target**” samples. P-value and Fold Change are 0.10 and 1.5, respectively).
- Click “**Launch**” to do Volcano Plot Generator analysis.
- Select **File** for abundance data of significant metabolites (e.g., [abundance\\_for\\_metabolites\\_with\\_significance\\_and\\_foldchange.szf](#)). Then, click “**File**” bottom and **Discover**. Click “**Multomics Data Mapper**” to upload the data of abundance for significant metabolites to the Multomics Data Mapper” gadget.



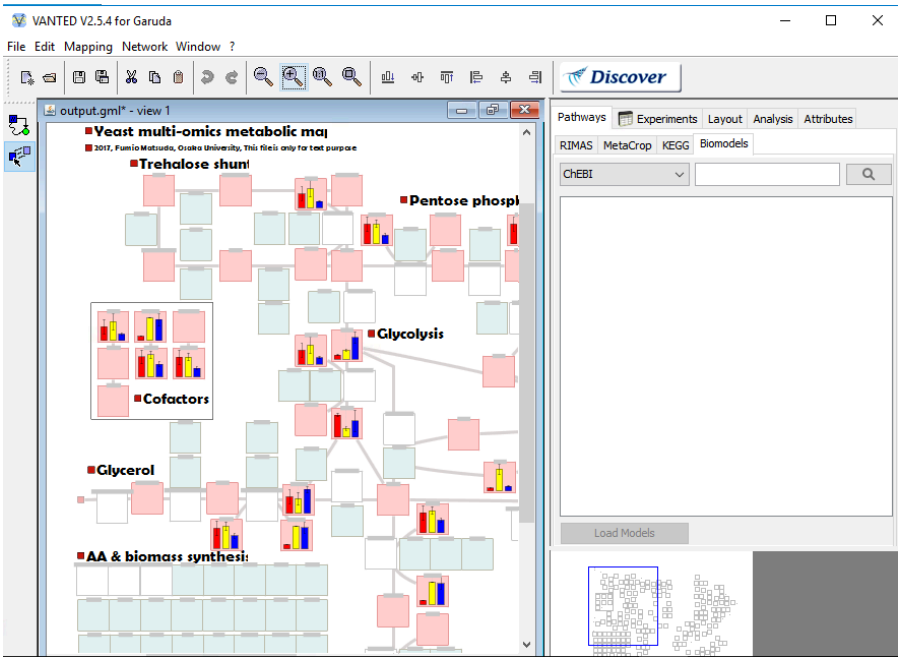


Metabolomics

**STEP 4. Visualize metabolome abundance data on metabolic network through VANTED.**

On clicking **Discover** in the last action in STEP3, a list of gadgets which can process merged gml file are displayed.

- 1. Select **VANTED** gadget and double click to launch VANTED gadget.  
Garuda will send the merged gml file to VANTED and open it for visualization.



# Recipe #1 : Visualize Metabolite Data to Metabolomic Pathway

## Metabolomics

**STEP 5.** Select significant metabolite list from Volcano Plot Generator analysis results and send the list to other gadget

1. Back to results from “**Volcano Plot Generator**” in STEP 2. analysis.
2. Select **File** for statistics for significant metabolites (e.g., `statistics_for_metabolites_with_significance_and_foldchange.txt`).
3. Then, click “**Data**” bottom and select column “**kegg id**”.
4. Click **Discover** and you can find “**iPath**” gadget.  
Click “**iPath**” to upload the list of significant metabolites on The “iPath” gadget to map the metabolites on kegg pathway.

**Volcano Plot Generator**

Input Files    Output Files

**abundance\_for\_metabolites\_with\_foldchange.szf**  
abundance\_for\_metabolites\_with\_foldchange.szf

**abundance\_for\_metabolites\_with\_significance.szf**  
abundance\_for\_metabolites\_with\_significance.szf

**abundance\_for\_metabolites\_with\_significance\_and\_foldchange.szf**  
abundance\_for\_metabolites\_with\_significance\_and\_foldchange.szf

**log.txt**  
log.txt

**statistics\_all.txt**  
statistics\_all.txt

**statistics\_for\_metabolites\_with\_foldchange.txt**  
statistics\_for\_metabolites\_with\_foldchange.txt

**statistics\_for\_metabolites\_with\_significance.txt**  
statistics\_for\_metabolites\_with\_significance.txt

**statistics\_for\_metabolites\_with\_significance\_and\_foldchange.txt**  
statistics\_for\_metabolites\_with\_significance\_and\_foldchange.txt

**VolcanoPLOT.pdf**  
VolcanoPLOT.pdf

Process finished successfully

**Discover**    **Data**    ?

"compound Name"	"kegg id"	"t-statistic"	"p-value"
STP	C05382	5.75223390550665	0.0143
FBP	C00354	-1.23453176614498	0.3412
XuSP	C00231	2.23845228551692	0.1094
RuSP	C00199	1.8989450844069	0.1399
RSP	C00117	1.73578103071007	0.2058
DHAP	C00111	2.02116156582944	0.1629
FGP	C00085	13.9436385517531	0.0003
AcCoA	C00024	-3.5108993421504	0.0355
NADP	C00006	-4.99713933482045	0.0142
NADH	C00004	14.273933755292	0.0048
NAD	C00003	-2.81964998858965	0.0585
ATP	C00002	-3.40547532412625	0.0628

Rescript volcano\_plot.r merge20170603002238.szf    Launch

**Volcano**

Input Files    Output Files

**abundance\_for\_metabolites\_with\_foldchange.szf**  
abundance\_for\_metabolites\_with\_foldchange.szf

**abundance\_for\_metabolites\_with\_significance.szf**  
abundance\_for\_metabolites\_with\_significance.szf

**abundance\_for\_metabolites\_with\_significance\_and\_foldchange.szf**  
abundance\_for\_metabolites\_with\_significance\_and\_foldchange.szf

**statistics\_all.txt**  
statistics\_all.txt

**statistics\_for\_metabolites\_with\_foldchange.txt**  
statistics\_for\_metabolites\_with\_foldchange.txt

**statistics\_for\_metabolites\_with\_significance.txt**  
statistics\_for\_metabolites\_with\_significance.txt

**statistics\_for\_metabolites\_with\_significance\_and\_foldchange.txt**  
statistics\_for\_metabolites\_with\_significance\_and\_foldchange.txt

**VolcanoPLOT.pdf**  
VolcanoPLOT.pdf

Process finished successfully

**Discover**    **Data**    ?

"compound Name"	"kegg id"	"t-statistic"	"p-value"
FBP	C00085	13.9436385517531	0.0003
NADH	C00004	14.273933755292	0.0048
NADP	C00006	-4.99713933482045	0.0142
STP	C05382	5.75223390550665	0.0143
AcCoA	C00024	-3.5108993421504	0.0355
NAD	C00003	-2.81964998858965	0.0585
ATP	C00002	-3.40547532412625	0.0628

Rescript volcano\_plot.r merge20170603002238.szf    Launch

Process finished successfully

**Gadgets**

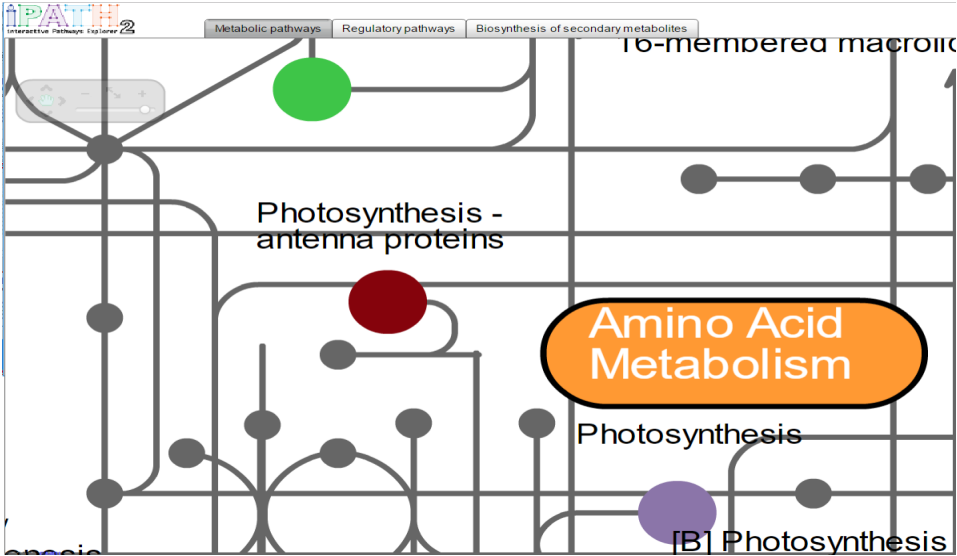
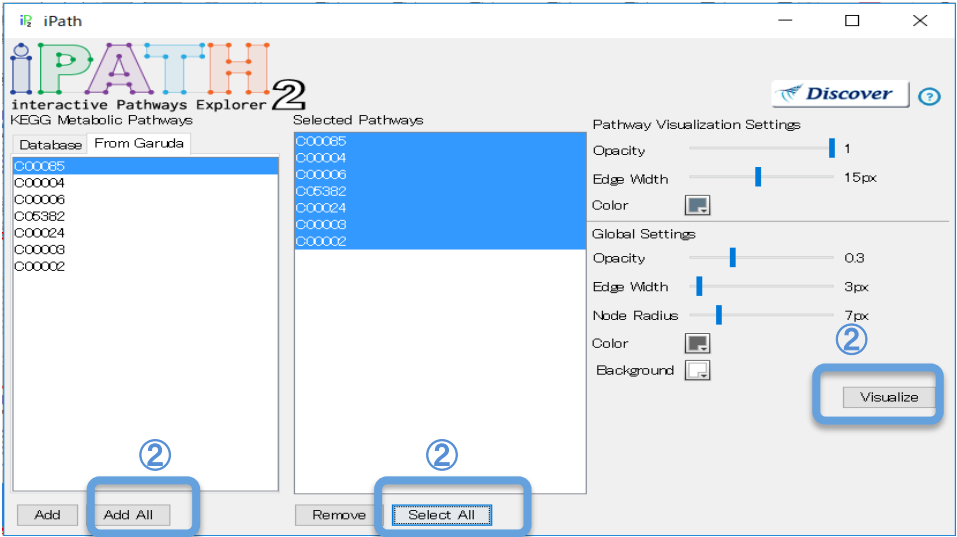
**iPath**

Close on Disconnect

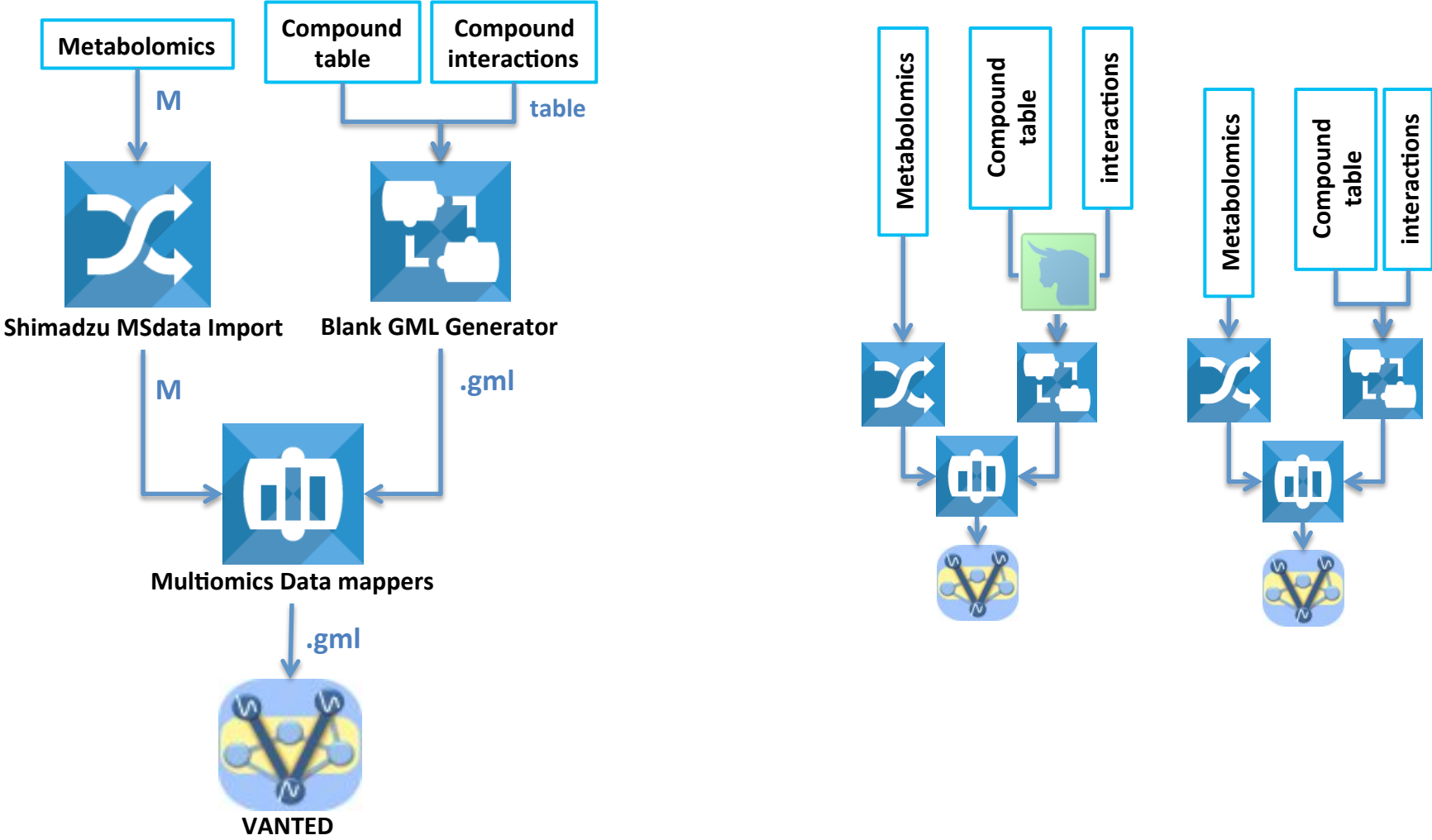
Metabolomics

Step 6. Mapping significant compounds on KEGG pathway map

1. On clicking **Discover** in the last action in STEP 5, a list of gadgets which can compounds list displayed. Select and double-click the “iPath” gadget. Garuda will launch the gadget and send the compounds name list to the gadget
2. Click “add all” and “select all” button to select all metabolites in the uploaded list.
3. Then, please click “visualize” button to map and visualize compounds on the KEGG pathway map.



Generate blank .gml file (metabolic network) from a list of compounds, and merge metabolite abundance data with the generated blank .gml file to visualize the abundance data on the metabolic network.





# Recipe #2 : Visualize Metabolite Data to Metabolomic Pathway on VANTED

Generate blank .gml file (metabolic network) from a list of compounds, and merge metabolite abundance data with the generated blank .gml file to visualize the abundance data on the metabolic network.

## Input

- **Metabolite quant data**  
(from LabSolutions Insight)  
<http://www.shimadzu.com/an/data-net/labsolutions/insight/index.html>
- **Compound List**
- **Compound Interactions**



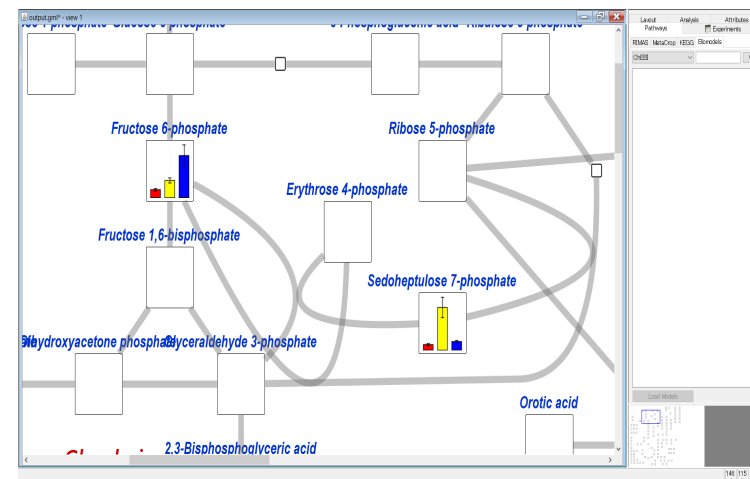
## Gadgets for Cooking Data



Nandi

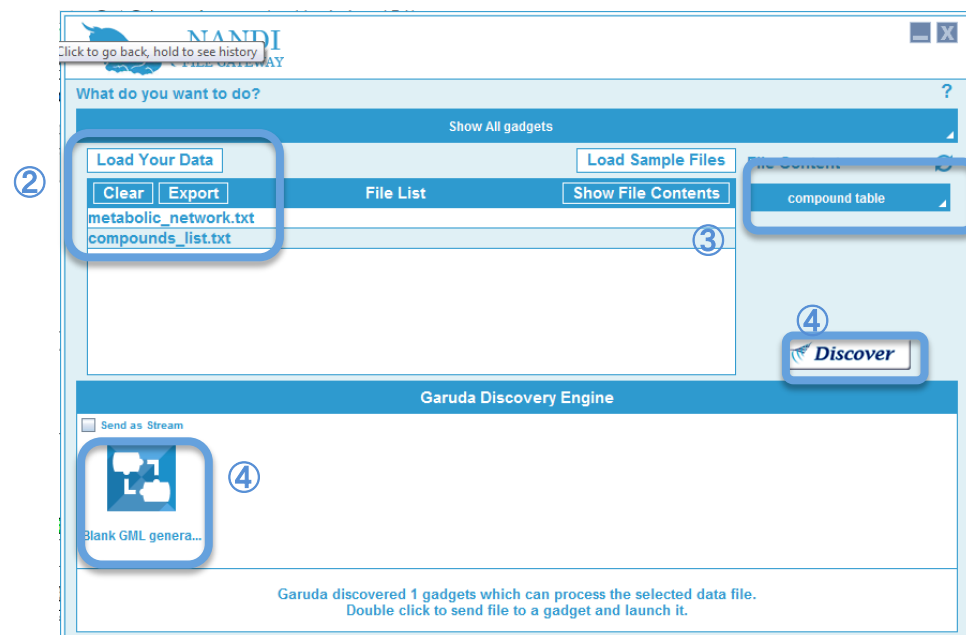


## OUTPUT



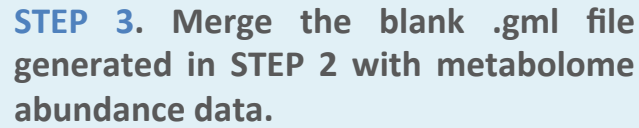
**STEP 1. Start with Nandi.**

1. Launch the gadget **Nandi** from the Garuda Dashboard (available under StartKit category).
2. Load the file sample compound list and the list of interactions between metabolites ("compounds\_list.txt" and "metabolic\_network.txt", respectively) from the local folder into **Nandi** and select it (in [ShimadzuGadgets\\_SampleData>BlankGMLGenerator](#)).
3. Choose "**compound table**" and "**kegg network**" for compound list and list of interactions between metabolites, respectively, from the content menu.
4. Press **Discover** button.
  - As Nandi is the discovery engine, many gadgets are discovered which can process these files for analysis.
  - For this recipe, initially, we want to try "Blank GML generator" to generate blank .gml file. Select and double-click the "**Blank GML Generator**"





1. From the **Nandi** discovery panel, select and double-click the “**Blank GML Generator**” gadget. Garuda will launch the gadget and send the data files to the gadget
2. Click “**Launch**” to make blank .gml file.
3. Click **Discover**. You can find “Multiomics Data Mapper” gadget. Please click “**Multiomics Data Mapper**” to upload the generated .gml file to “Multiomics Data Mapper”.



- Multomics Data Mapper**

Input Files    Output Files

**Pathway GML File**  
black.gml

**Shimadzu Multi-omics Data**  
merges.fzf

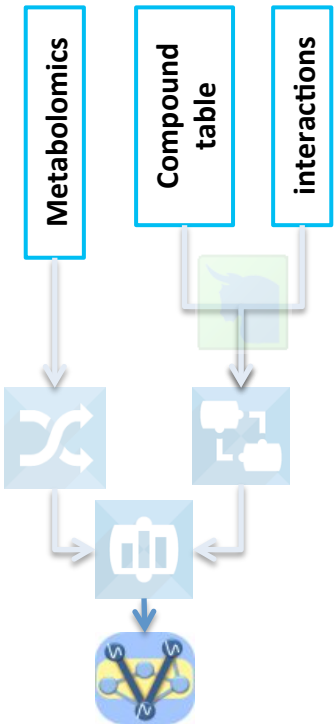
②

Name (Sample ID)	CHEBI	Inchi	kegg	S288C:S288C:S288C_1.m
GP	4170	NBSCHQZLSJFNQ-GASJEMHNSA-N	C00092	0.255
SP	52742	KTVPOYAKDPRIHY-SOOFDHINKSA-N	C00117	0.007
HP	48153	NGHMNDPNVRFEGS-IUYGOCFVISA-N	C00279	0.046
S/P	15721	JDTUMPKOJBQPKL-GBNDHIKLSA-N	C05382	0.029
P/R	32816	LCTONWCANYUPML-UHFFFAOYSA-N	C00022	0.806
DHAP	16108	GNGACRATGGDKBX-UHFFFAOYSA-N	C00111	0.042
AMP	16027	UDMBCSSLTHNCD-KQYNXICUSA-N	C00020	0.023
FBP	16905	XPYBSIWDXFQMNH-YUFOZJQFSA-N	C00354	5.428
3PG+2PG	17835	C00197	C00631	0.164
PEP	18021	DTBNBXWJWCVIC-UHFFFAOYSA-M	C00074	0.029
6PG	48928	BIRSGZKFOLSJQ-SQOUGZDYSA-N	C00345	0.073
ADP	16761	XYTWTFMLZFPYCI-KQYNXICUSA-N	C00008	0.012
ATP	15422	ZKHQWZAMYRWXGA-KQYNXICUSA-N	C00002	0.399
AcCoA	15351	ZSLZBFDCINBPY-ZSKIKINUSA-N	C00024	0.028
F6P	61553	BGWGXPPAYGQALX-VRPWFDPYSA-N	C00085	0.031
XuSP			C00231	0.008
RuSP	17363	FNZLKVNWIIPSJ-LHNWVWZDZSA-N	C00199	0.002
NAD	15846	BAWFJGIZGEFAR-NNYOXOHSSA-O	C00003	0.112
NADP	18009	XJLJKNUKWONI-NNYOXOHSSA-O	C00006	0.042
NADH	16908	BOPGDNLIDQYTO-NNYOXOHSSA-N	C00004	0.006
NADPH	16474	ACFIJLJDZMPIO-NNYOXOHSSA-N	C00005	0.07

cmd /c perl Mapper.pl black.gml merge.szf

Launch

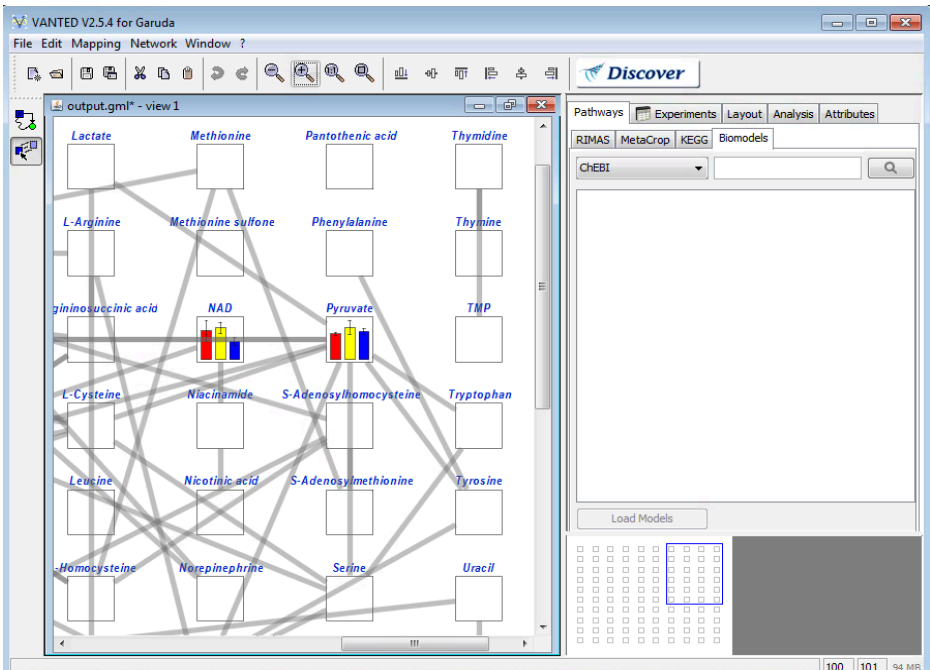
- Confidential



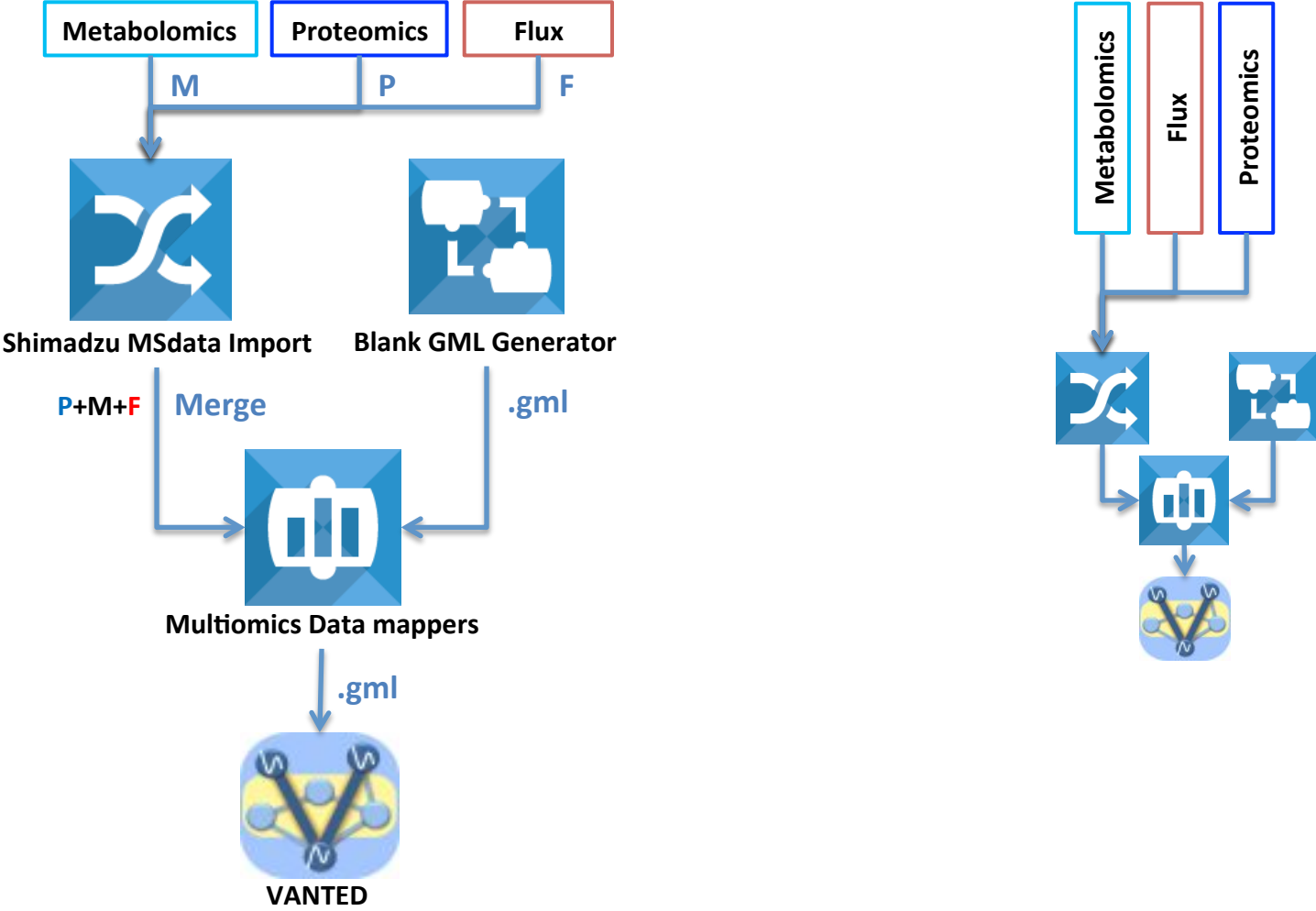
**STEP 4. Visualize metabolome abundance on blank metabolome network through VANTED.**

On clicking **Discover** in the last action in STEP3, a list of gadgets which can process merged .gml file are displayed.

- 1. Select **VANTED** gadget and double click to launch VANTED gadget. Garuda will send the merged .gml file to VANTED and open it for **visualization**.



Merge multi-omics data with the blank .gml file and visualize the multi-omics data on the molecular network.



Merge multi-omics data with the blank .gml file and visualize the multi-omics data on the molecular network.

Input

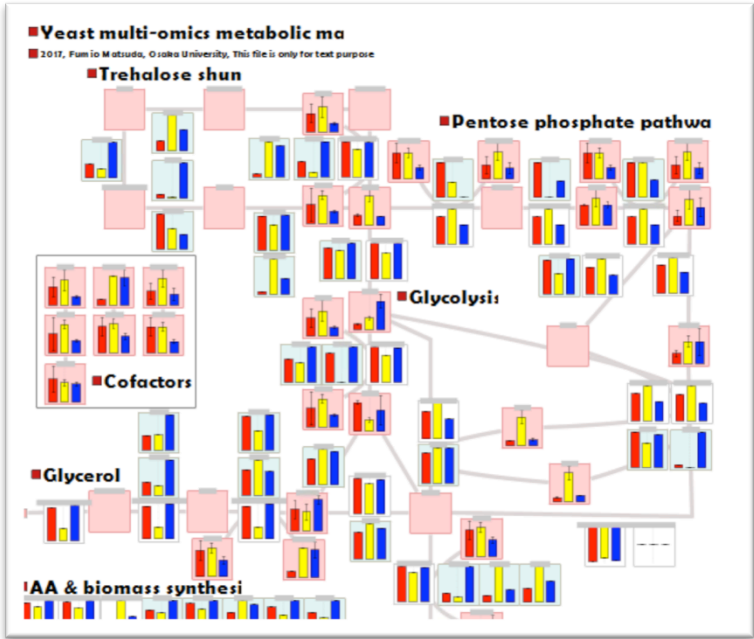
- **Metabolite quant data**  
(from LabSolutions Insight)  
<http://www.shimadzu.com/an/data-net/labsolutions/insight/index.html>
- **Proteomics quant data**  
(from Skyline)
- **Flux quant data**  
(from

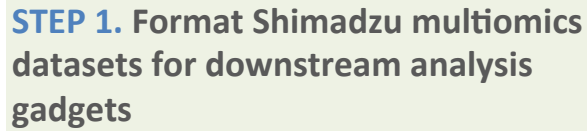


Gadgets for Cooking Data



OUTPUT





- Shimadzu MS data Import

File | Data | Filter

☐ Add Protein quant File(.csv)  
☒ Add Metabolite quant File(.csv)  
☐ Add Flux quant File(.csv)  
☐ Exit

☐ Merged by Sample No.  
☐ Merged by Sample  
☐ Avg. of timecourse

Output Style

☒ Table  
☐ List

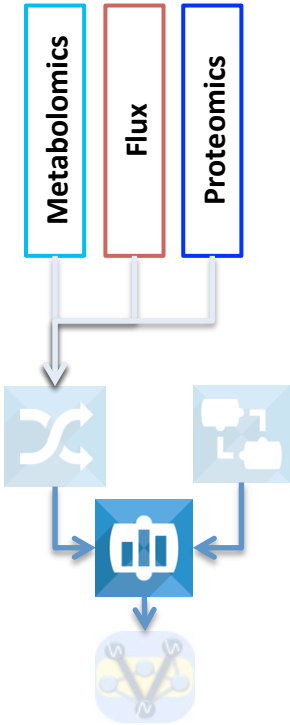
Load Initial Data

Clear Data

(Sample Name)	select	Name	CHEBI	Inchi	kegg	S288C-S288C_1,m	S288C-S288C_2,m	S288C-S288C_3,m	pkf.Delta	pkf.1,m	pkf.1c
(Sample ID)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	S288C	S288C	S288C	pkf.Delta	pkf.1,m	pkf.1c
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	0	0	0	0	0	0
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	0	0	0	0	0	0
1	<input checked="" type="checkbox"/>	G6P	4170	NBSCHOHZLSJ..	C00092	0.255	0.315	0.288	0.813	0.721	
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPIYQYAKDP.	C00117	0.007	0.01	0.008	0.022	0.017	
3	<input checked="" type="checkbox"/>	E4P	48153	NGHMNPNXVRF.	C00279	0.046	0.053	0.047	0.263	0.263	
4	<input checked="" type="checkbox"/>	S7P	15721	JDTUMPKOJBO.	C05392	0.029	0.030	0.032	0.234	0.24	
5	<input checked="" type="checkbox"/>	PYR	32816	LCTONMCANLY.	C00022	0.806	0.825	0.763	1.092	0.812	
6	<input checked="" type="checkbox"/>	DHAP	16108	GNQACRATGSD.	C00111	0.042	0.061	0.068	0.054	0.041	
7	<input checked="" type="checkbox"/>	AMP	16027	UDMBGSLSTHL..	C00020	0.023	0.017	0.01	0.015	0.015	
8	<input checked="" type="checkbox"/>	FBP	16905	XPYBSWDXQFN.	C00354	5.428	5.214	4.981	1.916	1.755	
9	<input checked="" type="checkbox"/>	3PG-2PG	17835	C00197	C00631	0.164	0.225	0.17	0.201	0.206	
10	<input checked="" type="checkbox"/>	PEP	18021	DTENBWJWCW.	C00074	0.029	0.039	0.026	0.043	0.046	
11	<input checked="" type="checkbox"/>	6PG	48928	BIFSGZFKXLS..	C00345	0.073	0.075	0.073	0.092	0.078	
12	<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY.	C00048	0.012	0.054	0.034	0.053	0.044	
13	<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW.	C00002	0.399	0.639	0.313	0.609	0.434	
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFCDGBIN.	C00024	0.028	0.045	0.024	0.043	0.031	
15	<input checked="" type="checkbox"/>	F6P	61553	BGGWG/PAPYGG.	C00085	0.031	0.025	0.03	0.061	0.058	
16	<input checked="" type="checkbox"/>	Xu5P			C00231	0.008	0.013	0.012	0.023	0.02	
17	<input checked="" type="checkbox"/>	Ru5P	17863	FNZUKVNUMBPS.	C00199	0.002	0.005	0.005	0.012	0.008	
18	<input checked="" type="checkbox"/>	NAD	15846	BAWFJGJZGEF.	C00003	0.112	0.169	0.112	0.144	0.162	

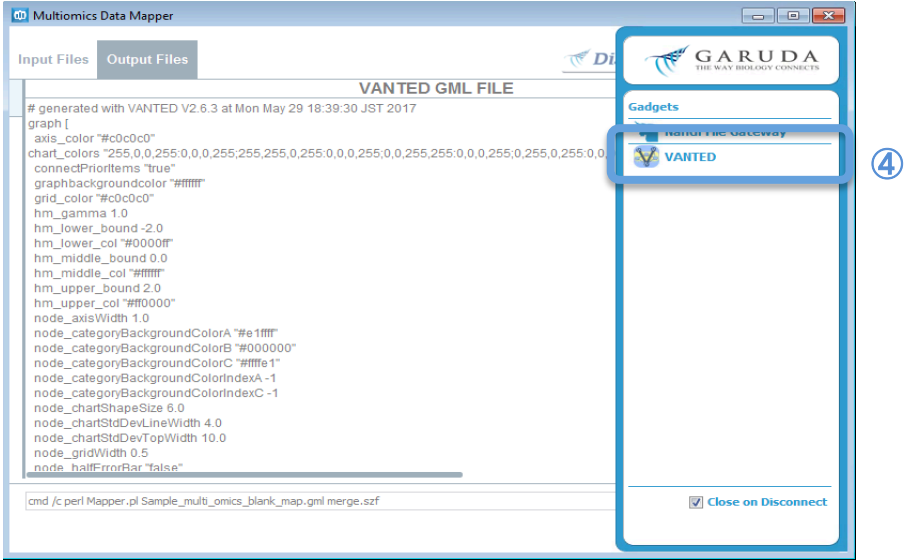
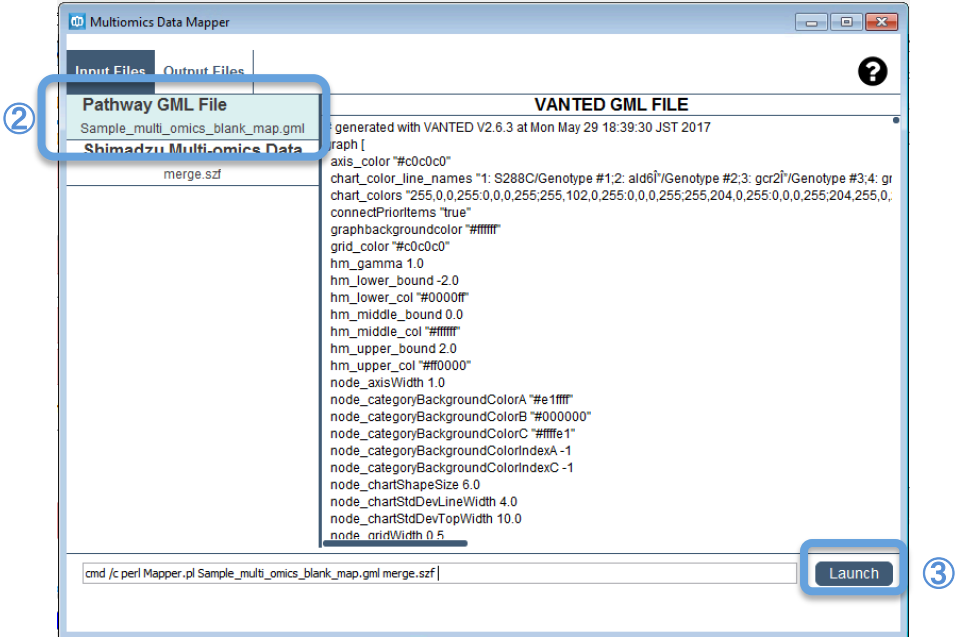


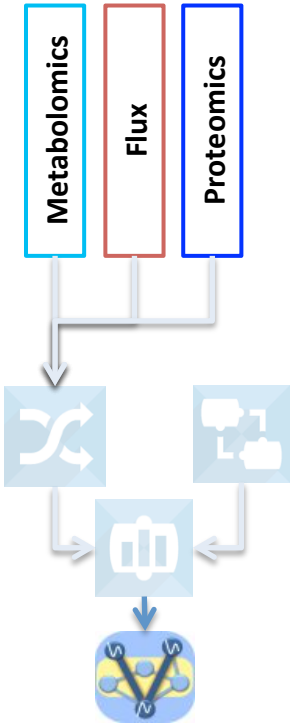




STEP 2: Merge multi-omics data on blank molecular network

1. From “**Shiamdzu MSdata Import**”, select and double-click the “**Multiomics Data Mapper**” gadget. Garuda will launch the gadget and send the data files to the gadget
2. Click “**gml file**” to upload gml file for blank molecular network, “transomics\_plane\_map\_withID0125.gml” (in **ShimadzuGadgets\_SampleData>MultiomicsDataMapper**).
3. Click “**Launch**” to merge the multi-omics data with blank molecular network.
4. Select **File** and click **Discover**. You can find **VANTED** gadget.





**STEP 3. Visualize multi-omics data on blank molecular network through VANTED.**

On clicking **Discover** in the last action in Step 2, a list of gadgets which can process merged .gml file are displayed.

- 1. Select **VANTED** gadget and double click to launch VANTED gadget. Garuda will send the merged .gml file to VANTED and open it for **visualization**.

