POWERED BY GARUDA

Shimadzu multi-omics data analysis

Tutorial

2017 July

SHIMADZU Excellence in Science

大阪大学 OSAKA UNIVERSITY

SBI The Systems Biology Institute

Contents

Release Date
2017 July

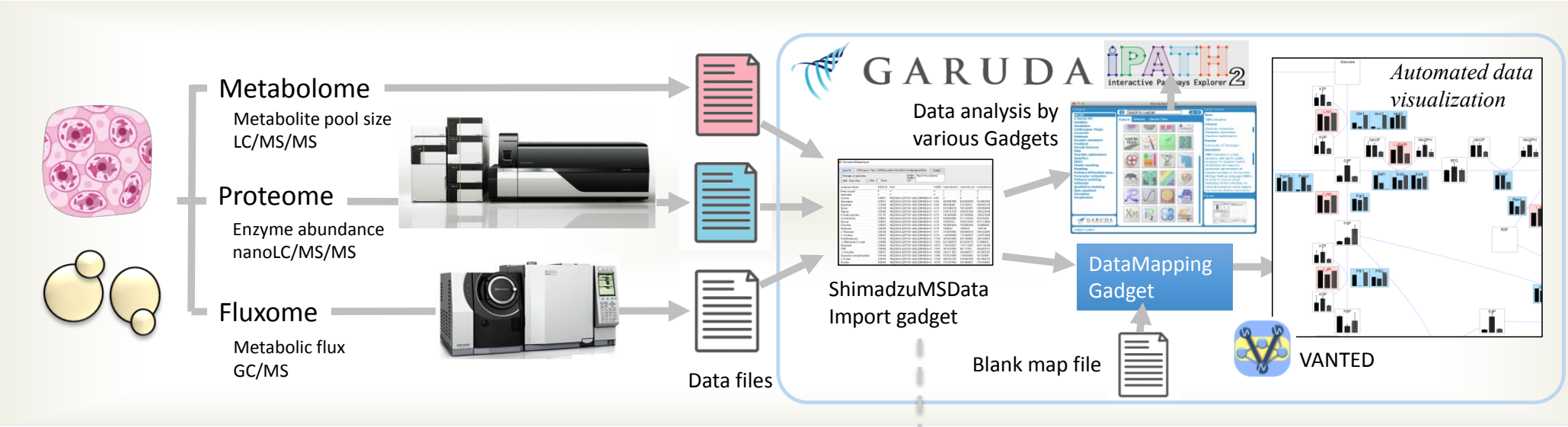
Contact
For queries, comments and feedback on specific Shimadzu multi-omics analysis gadgets, please mail us at info@sbx-corp.com
For Garuda community gadgets, please send email to garudahelpline@gmail.com

Garuda™

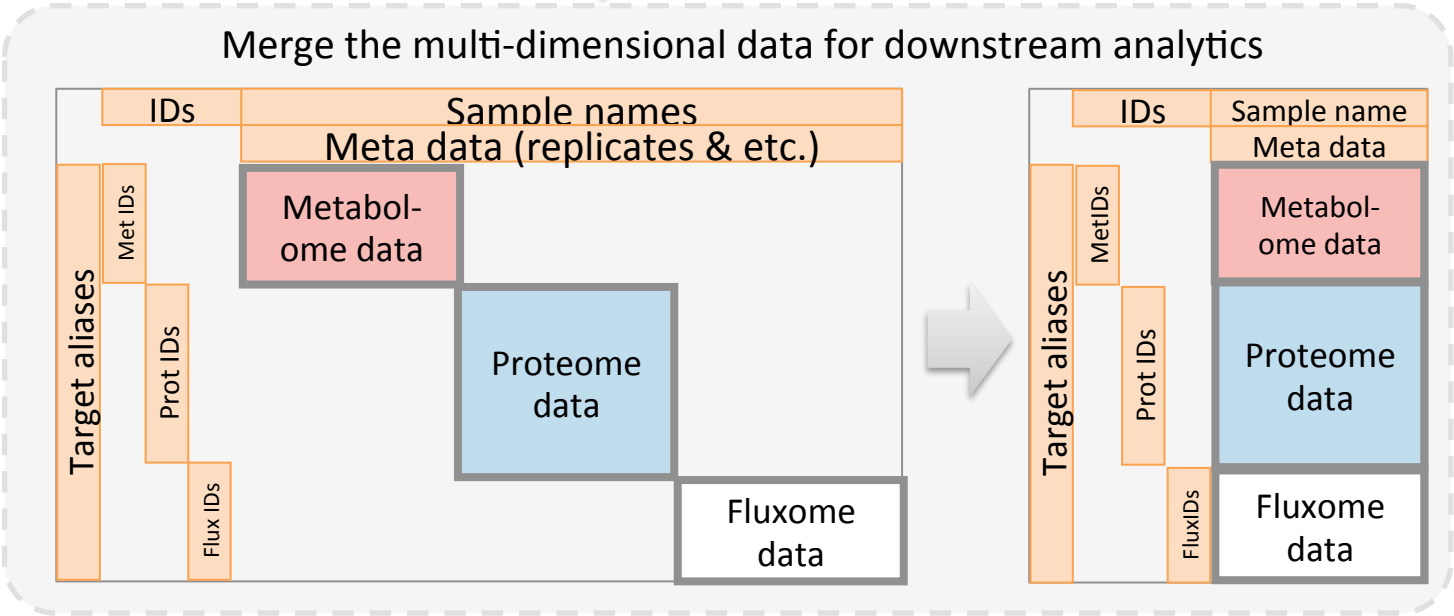
What's New ver1.0.1

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

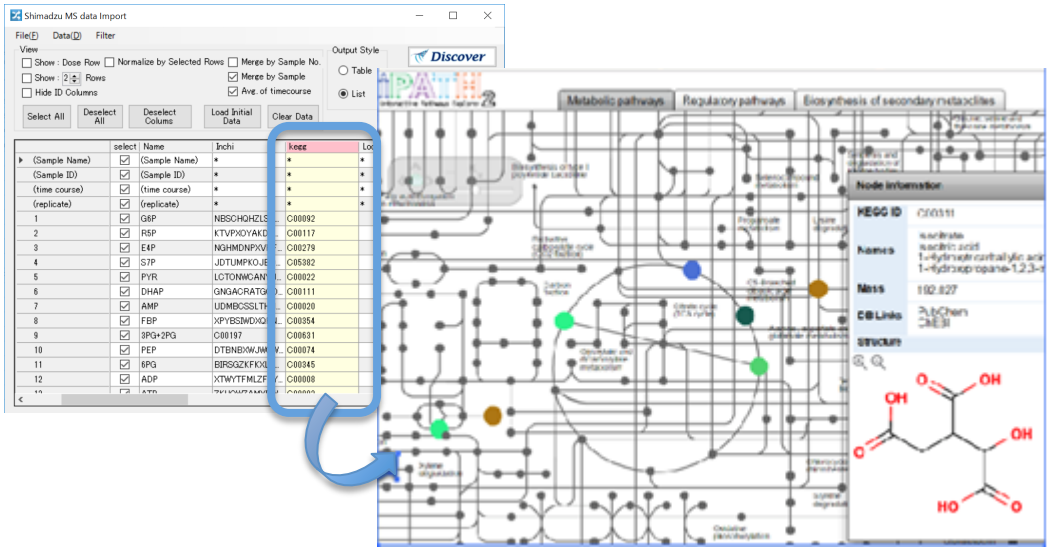
What is the Shimadzu multi-omics data analysis?



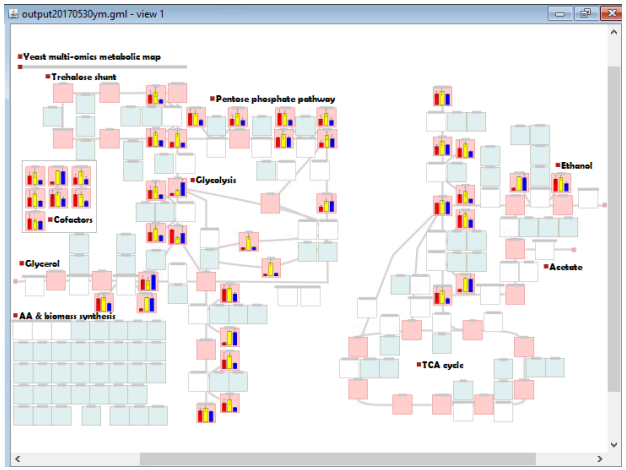
"**Shimadzu Multi-Omics Analysis Pack**" can automatically process, analyze proteomics, metabolomics, and flux data obtained by Shimadzu's gas chromatograph mass spectrometer (GCMS) and liquid chromatography mass spectrometer (LCMS) and visualize the results on pathway maps.

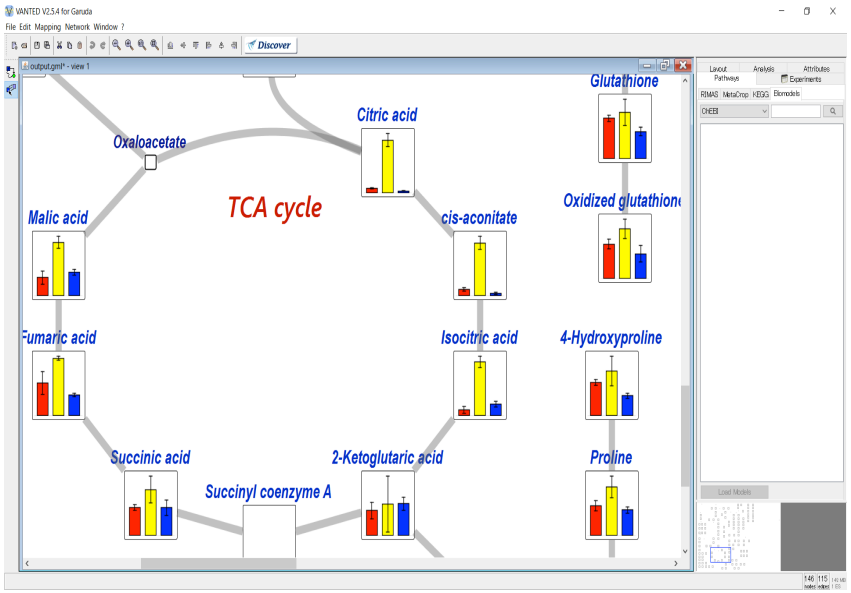


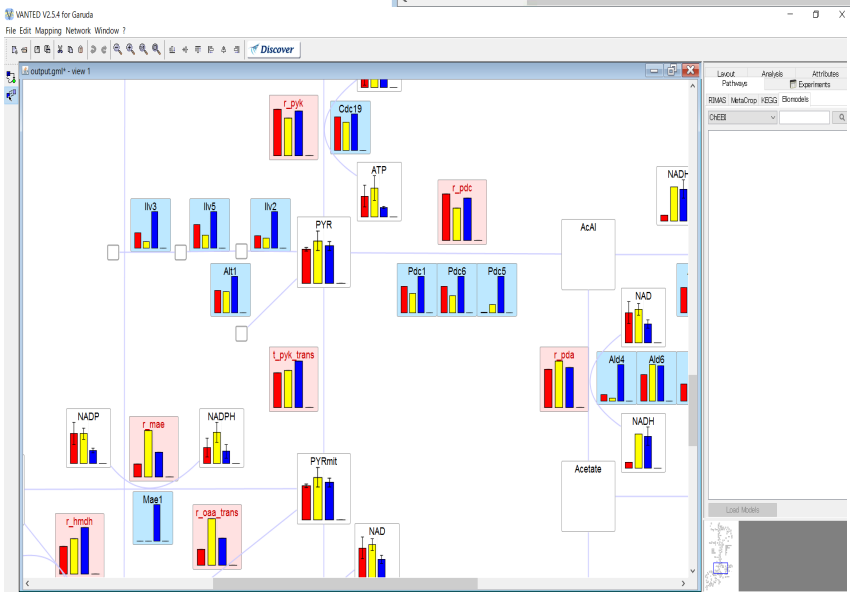
Shimadzu multi-omics analysis visualization



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

"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.

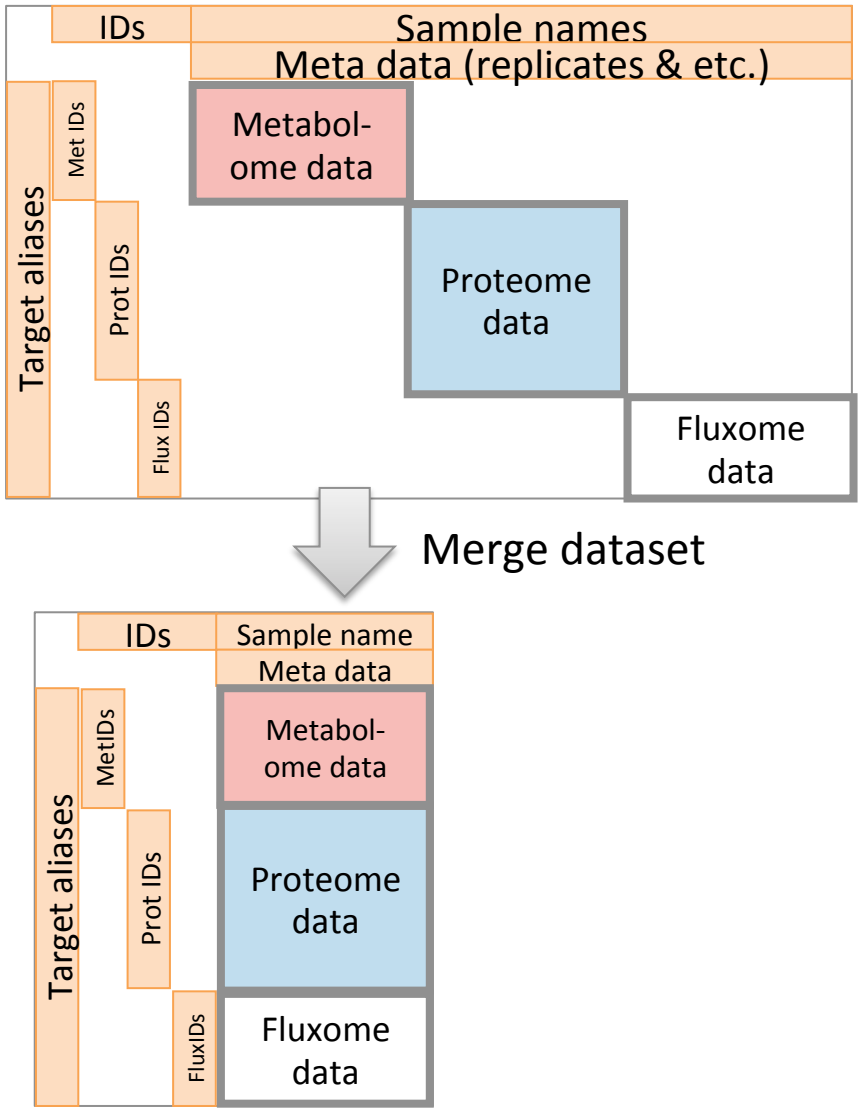
INPUT
- Metabolite data
- Proteomics data
- Flux data

(.csv, .txt)

- **Merge dataset**
- **Normalize data**
- **Average timecourse data**
- **Impute data**
- **Select compounds**

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

(.szf)



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

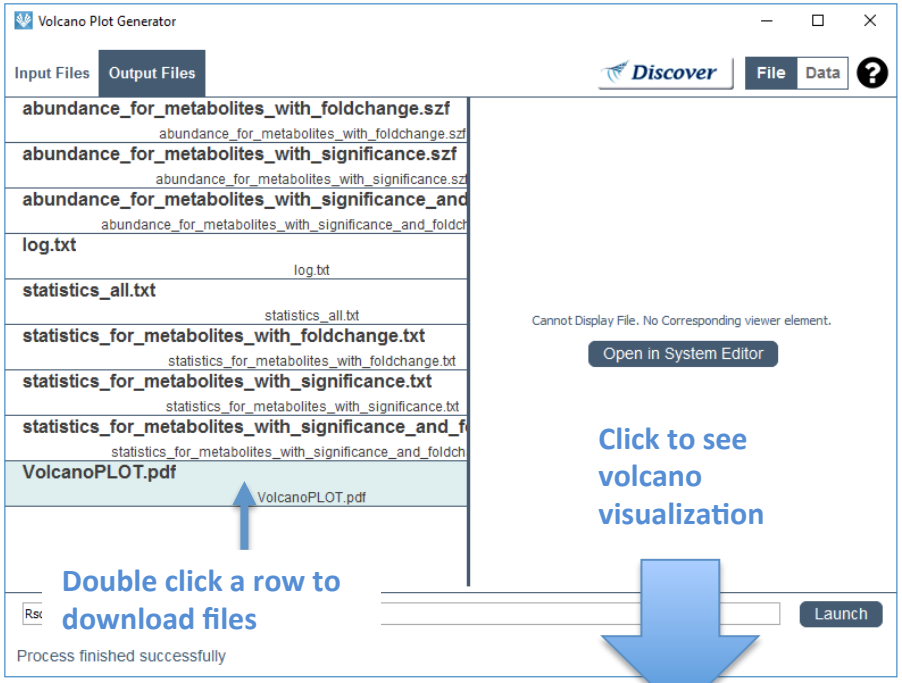
(.csv)

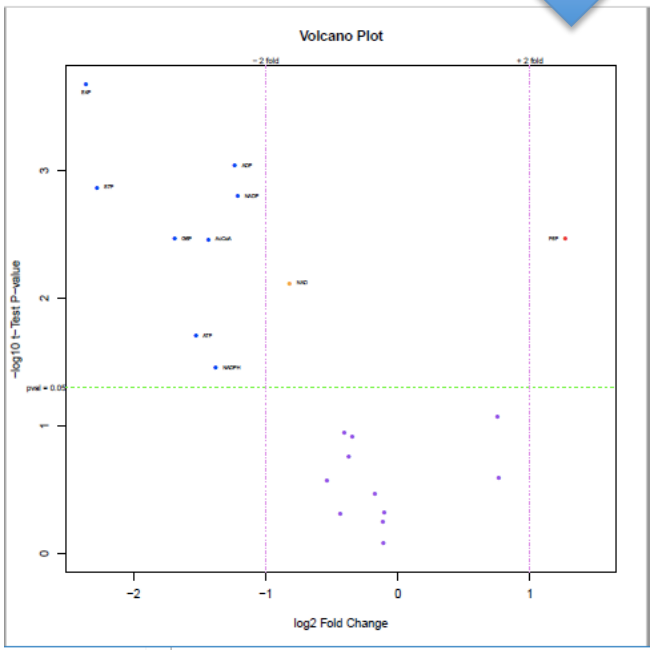
- **Volcano Plot Generator analysis for metabolome abundance**

OUTPUT

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

(.szf)





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

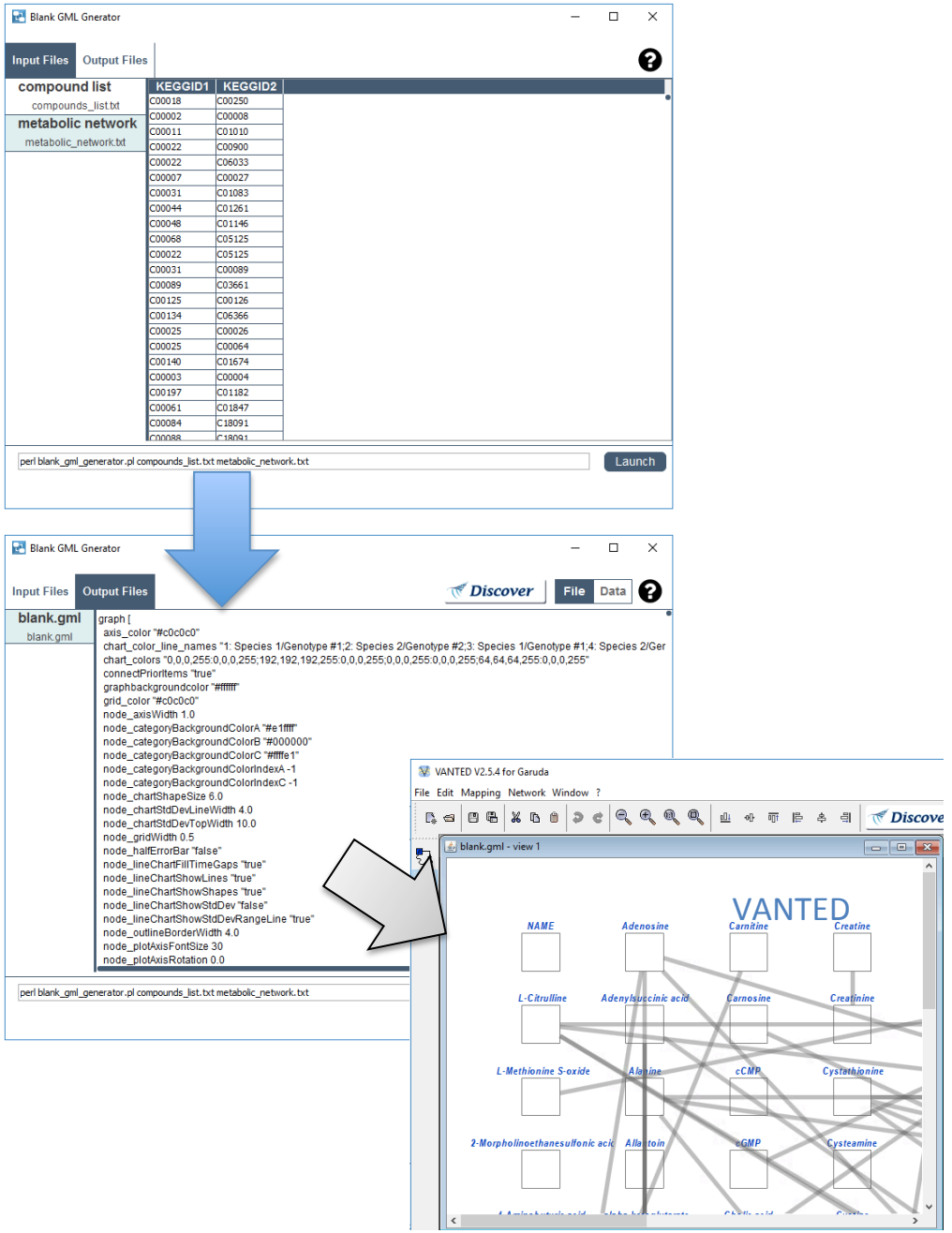
(.csv)

- **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

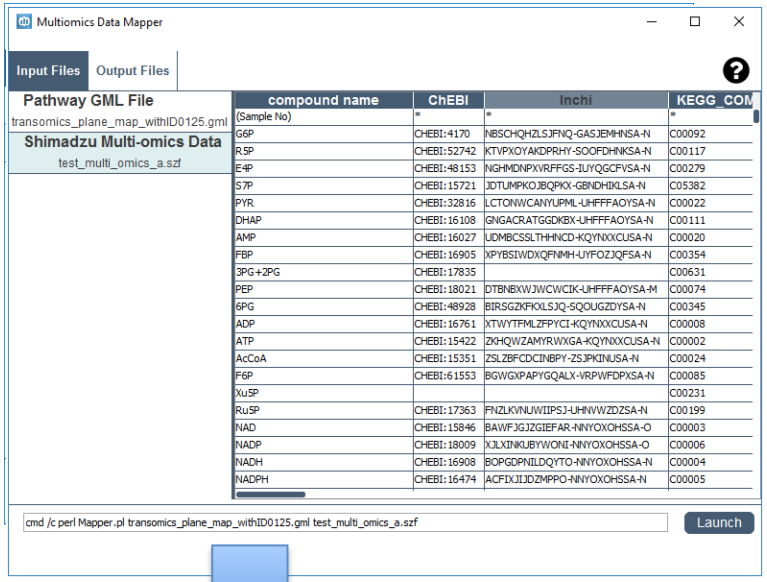
(.gml)

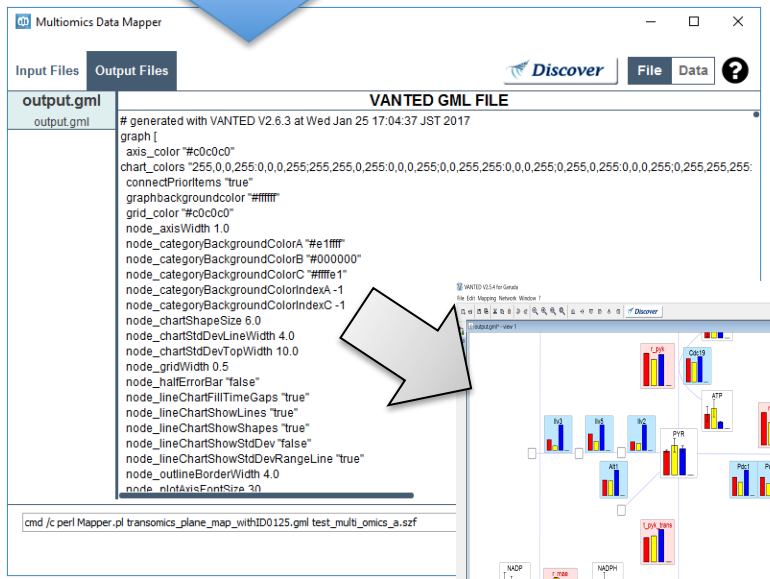
- **Merge Shimadzu multi-omics data with .gml file for VANTED**

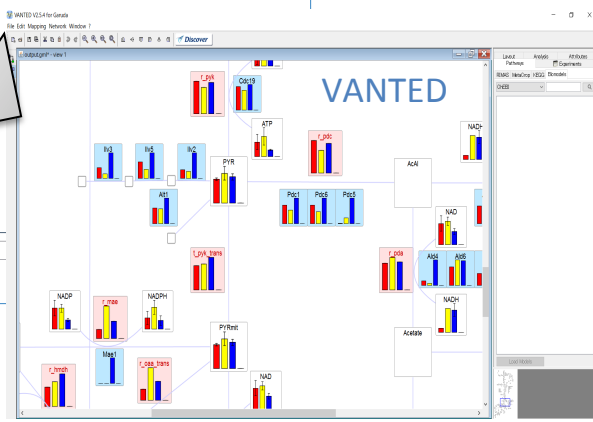
OUTPUT

- Send data to VANTED

(.gml)







Installation and Troubleshooting

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

Shimadzu MSdata Import

Volcano Plot Generator

Blank GML Generator

Multiomics Data Mapper

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.

INPUT

- Metabolite data
- Proteomics data
- Flux data

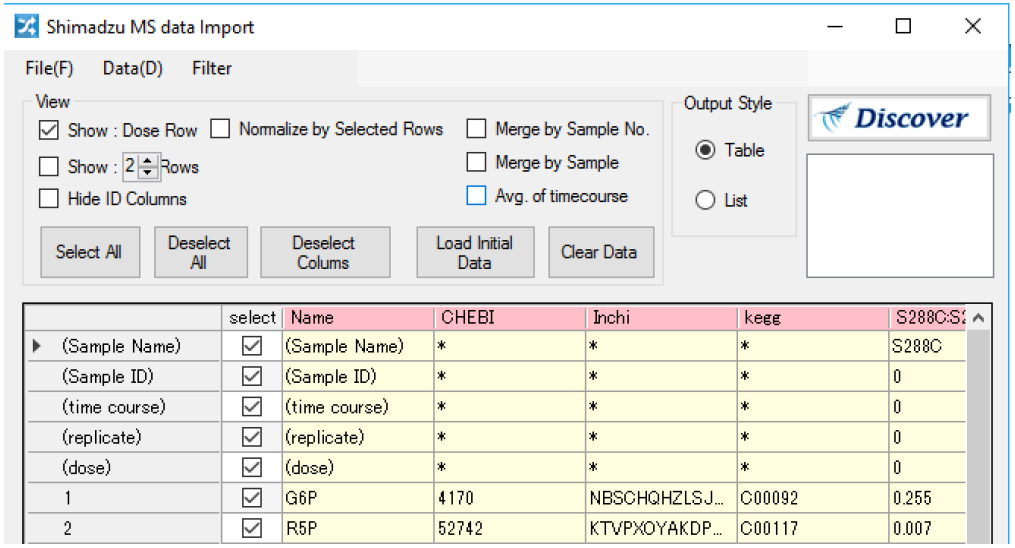
(.csv, .txt)

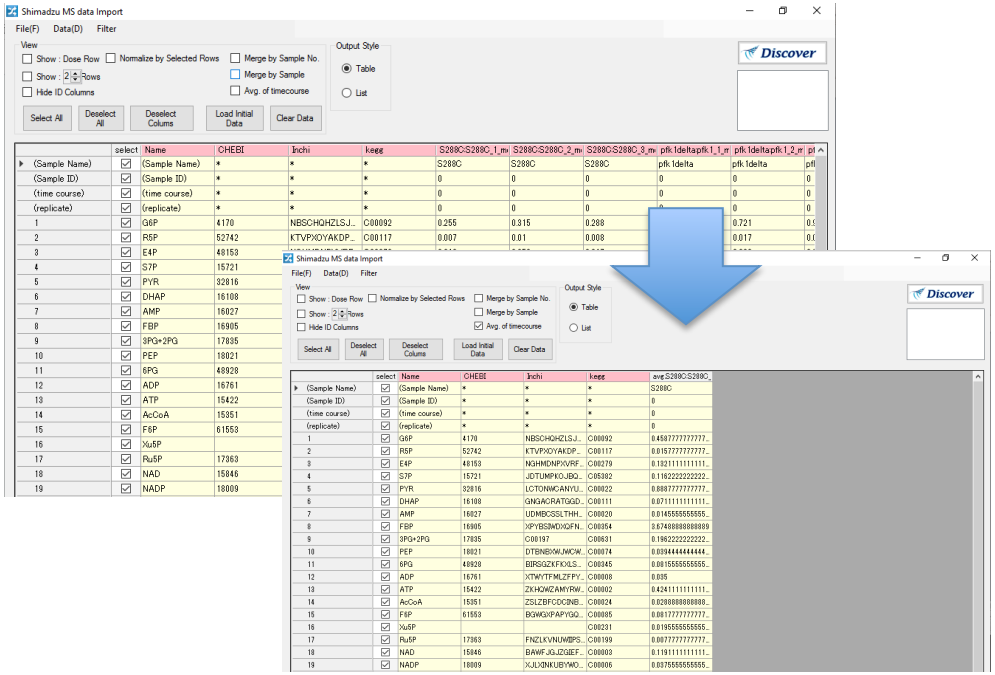
- **Clear Load Data**
- **Edit Data**
- **Imputate data**
- **Average timecourse data**
- **Merge dataset**
- **Select Output Style**

OUTPUT

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

(.szf)





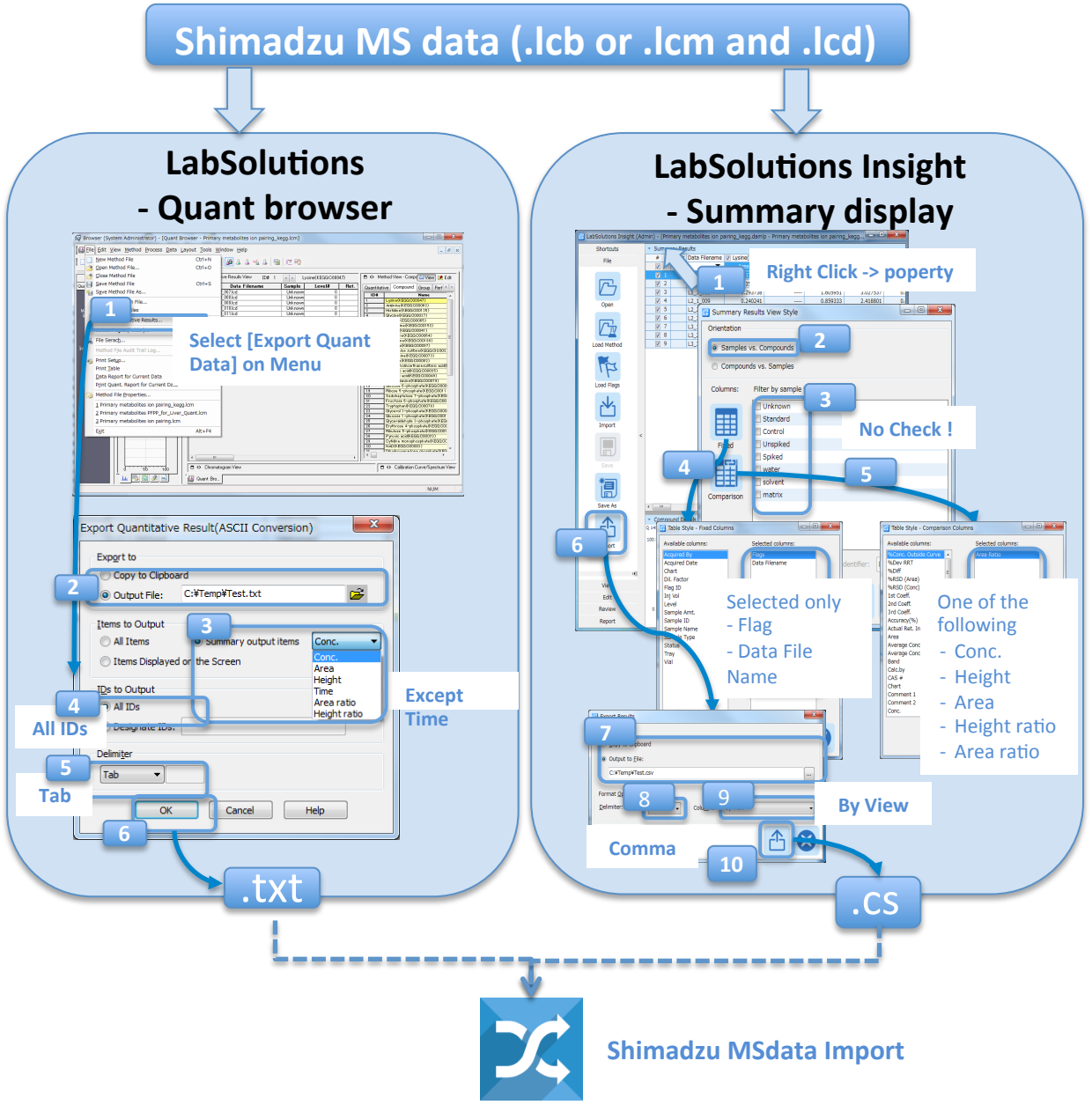
Shimadzu MSdata Import

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 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).

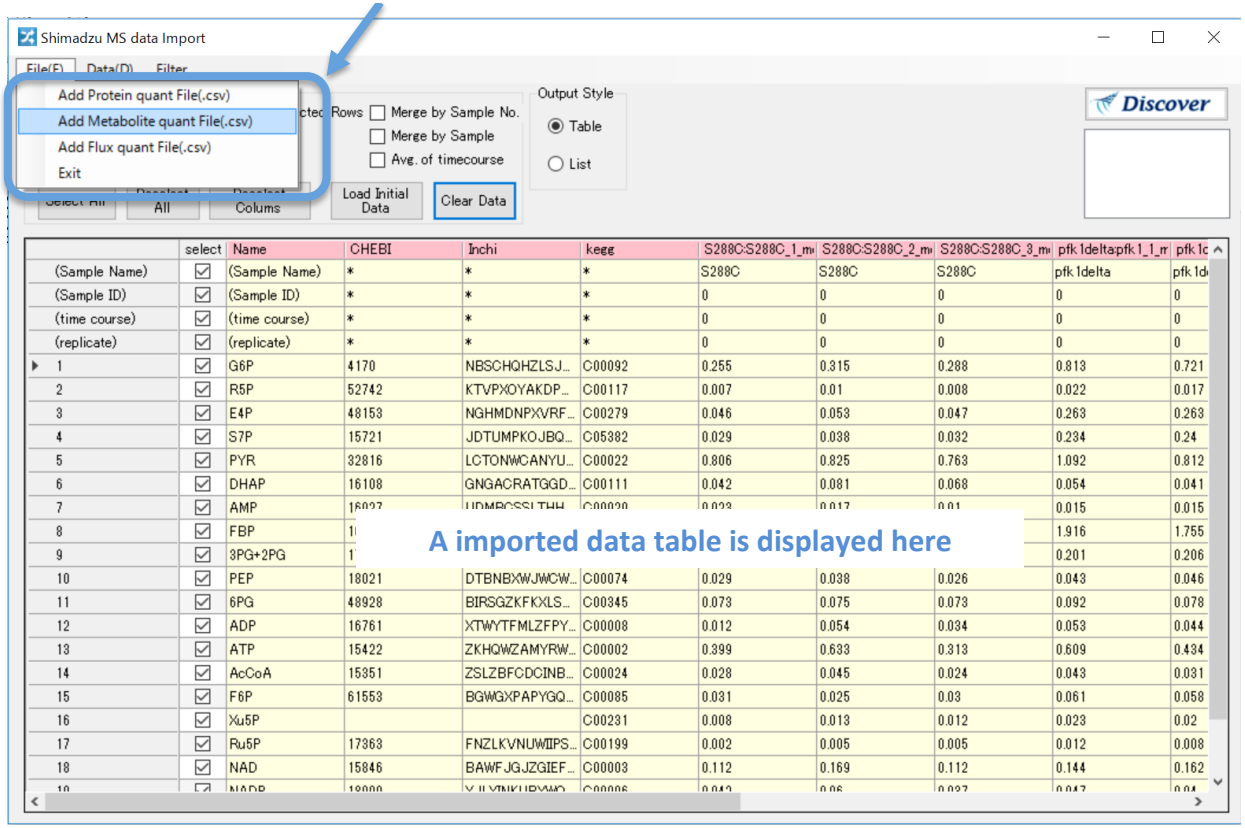
Note: if you select and load two different data files, the gadget merges the two selected files to make a single data table.

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



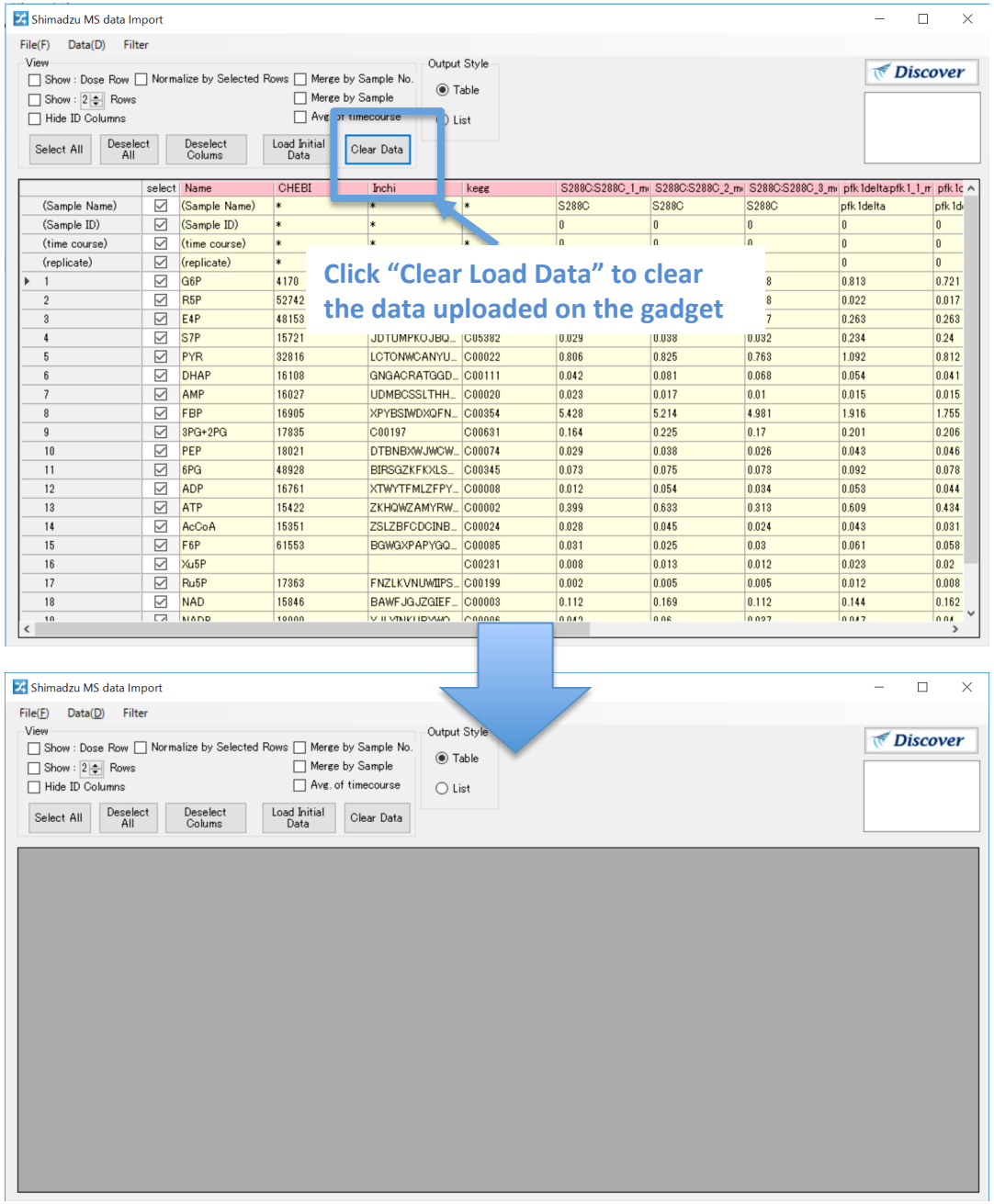
	select	Name	CHEBI	Inchi	kegg	S288C:S288C_1_m	S288C:S288C_2_m	S288C:S288C_3_m	pfk1delta:pfk1_1_m	pfk1c
(Sample Name)	☑	(Sample Name)	*	*	*	S288C	S288C	S288C	pfk1delta	pfk1d
(Sample ID)	☑	(Sample ID)	*	*	*	0	0	0	0	0
(time course)	☑	(time course)	*	*	*	0	0	0	0	0
(replicate)	☑	(replicate)	*	*	*	0	0	0	0	0
1	☑	G6P	4170	NBSCHQHZLSJ...	C00092	0.255	0.315	0.288	0.813	0.721
2	☑	R5P	52742	KTVPXOYAKDP...	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	JDTUMPKOJBQ...	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	GNGACRATGGD...	C00111	0.042	0.081	0.068	0.054	0.041
7	☑	AMP	16027	UDMBCSSLTHH...	C00020	0.023	0.017	0.01	0.015	0.015
8	☑	FBP	1						1.916	1.755
9	☑	3PG+2PG	1						0.201	0.206
10	☑	PEP	18021	DTBNBXWJWCW...	C00074	0.029	0.038	0.026	0.043	0.046
11	☑	6PG	48928	BIRSGZKFKXLS...	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	ZSLZBFCDCINB...	C00024	0.028	0.045	0.024	0.043	0.031
15	☑	F6P	61553	BGWGXPAPYGQ...	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	FNZLKVNUWIIPS...	C00199	0.002	0.005	0.005	0.012	0.008
18	☑	NAD	15846	BAWFJGJZGIEF...	C00003	0.112	0.169	0.112	0.144	0.162
19	☑	NADP	18009	XJLXINKUBYWG...	C00006	0.042	0.06	0.037	0.047	0.04

Shimadzu MSdata Import

Data Processing

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

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

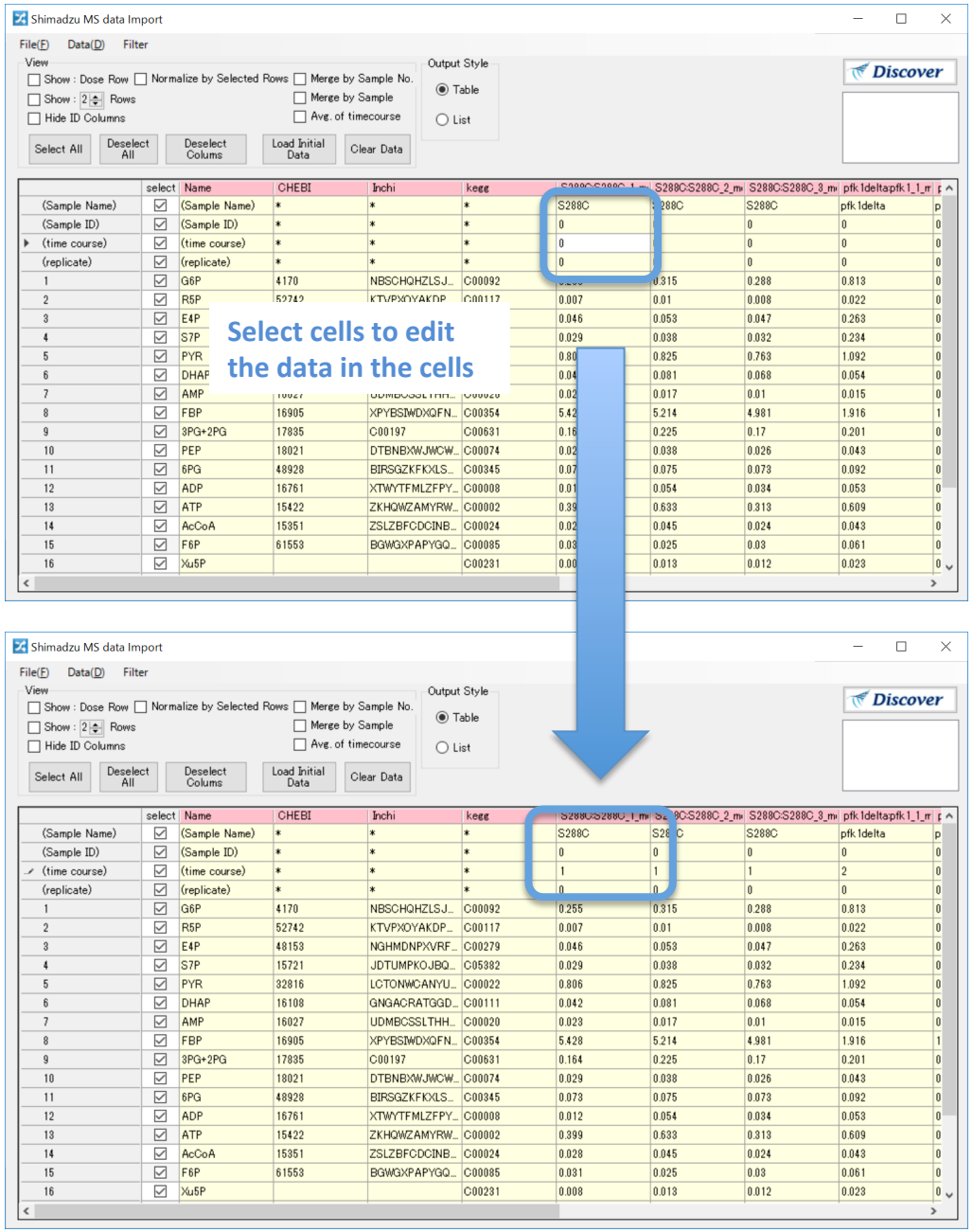


Shimadzu MSdata Import

Data Processing

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

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



Shimadzu MSdata Import

Data Processing

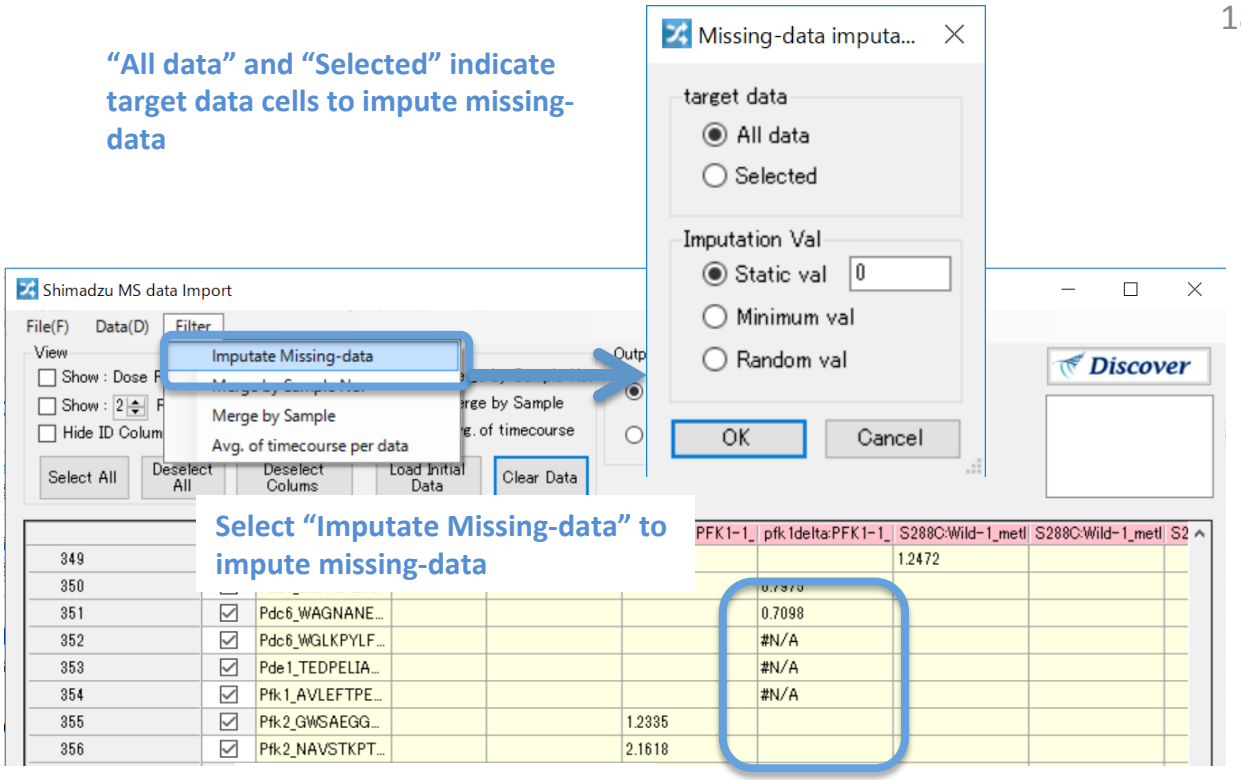
- Clear Load Data
- Edit Data
- **Imputate data**
- Average timecourse data
- Merge dataset
- Select Output Style

1. Select "**Imputate 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.

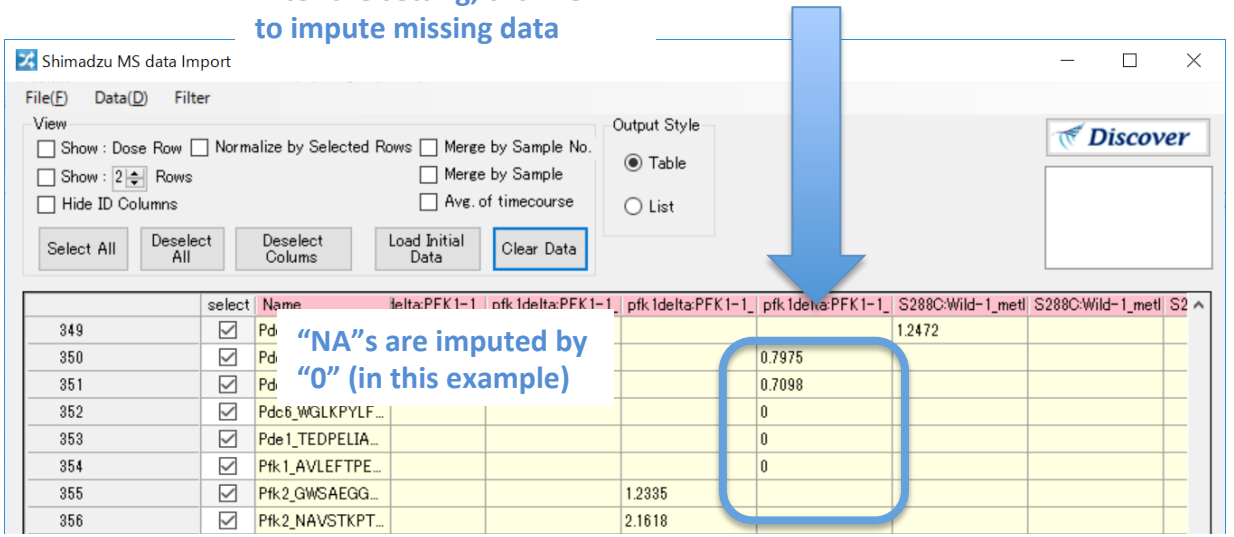
2. "**All data**" and "**Selected**" indicate target data cells (all cells and selected cell respectively) to impute missing-data.
   "**Static val**",
   "**Minimum val**", and
   "**Random val**",
   indicate a value (user defined value, minimum value in the data, value selected randomly from the data, 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



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

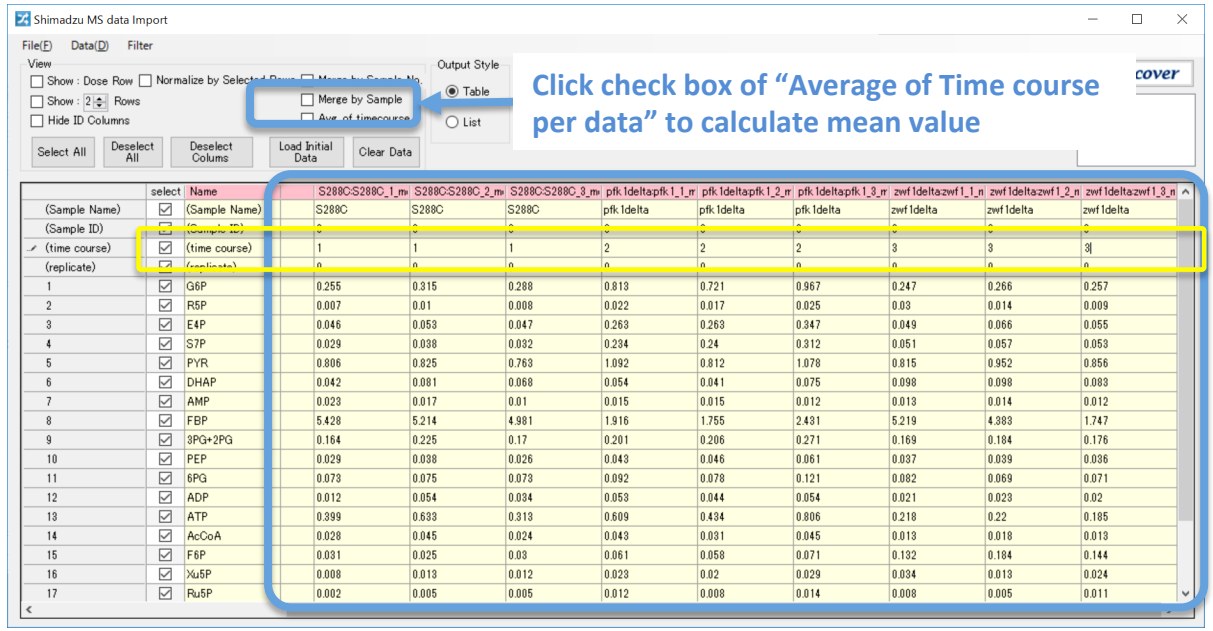


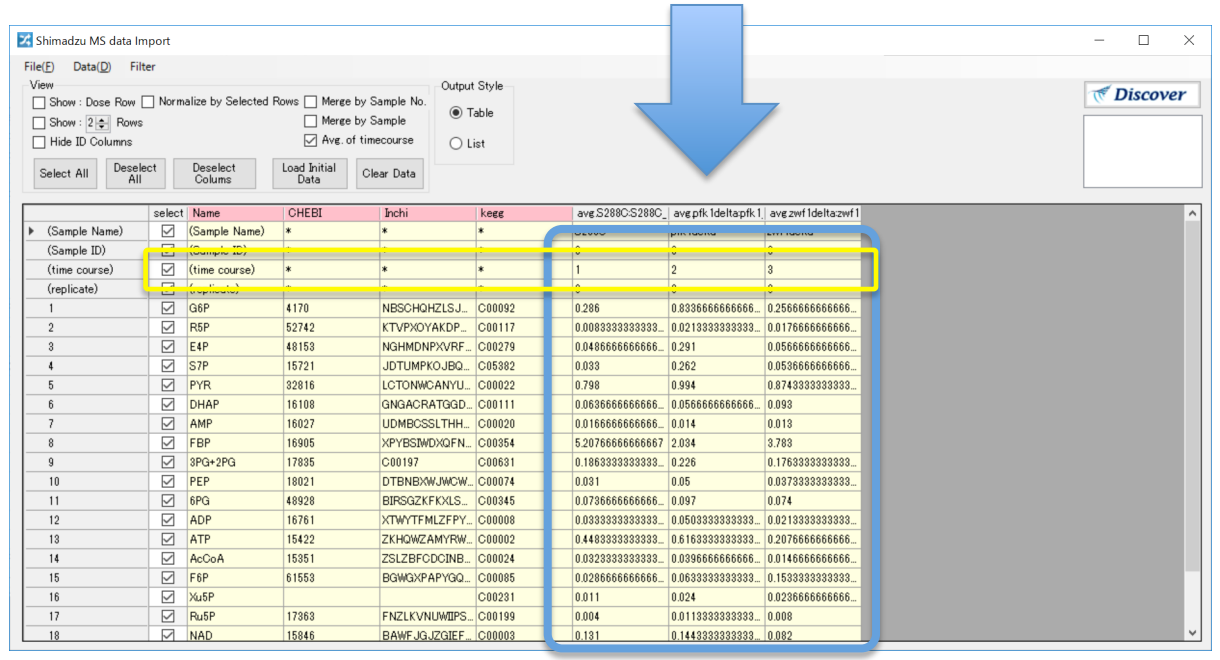
Shimadzu MSdata Import

Data Processing

- Clear Load Data
- Edit Data
- Imputate 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.



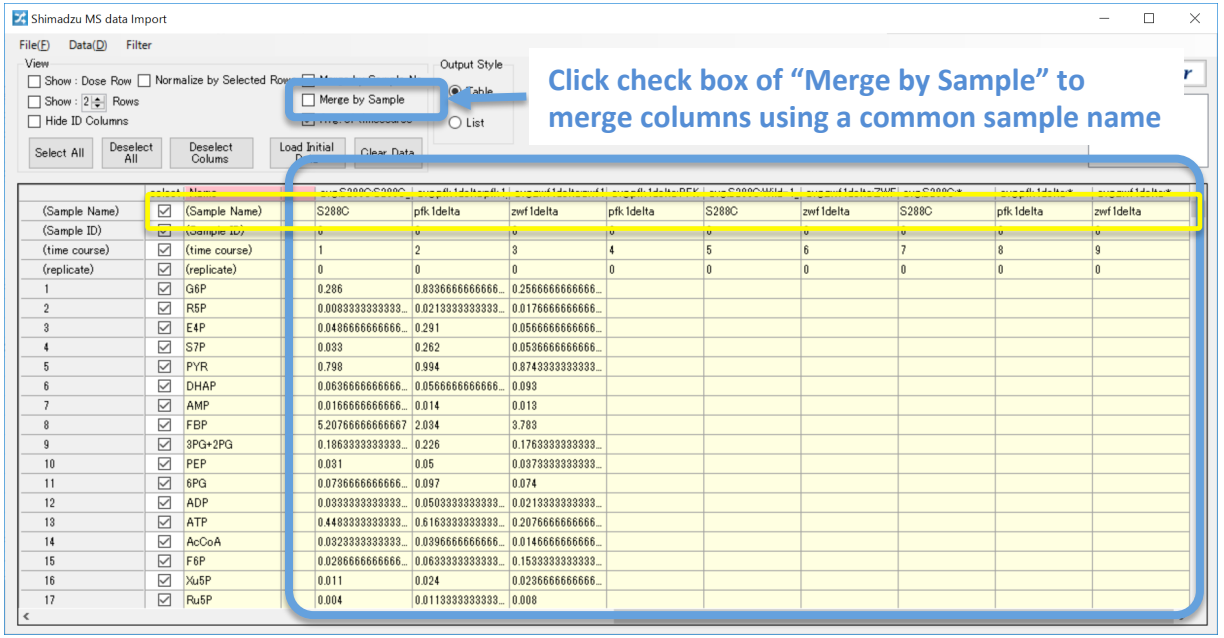


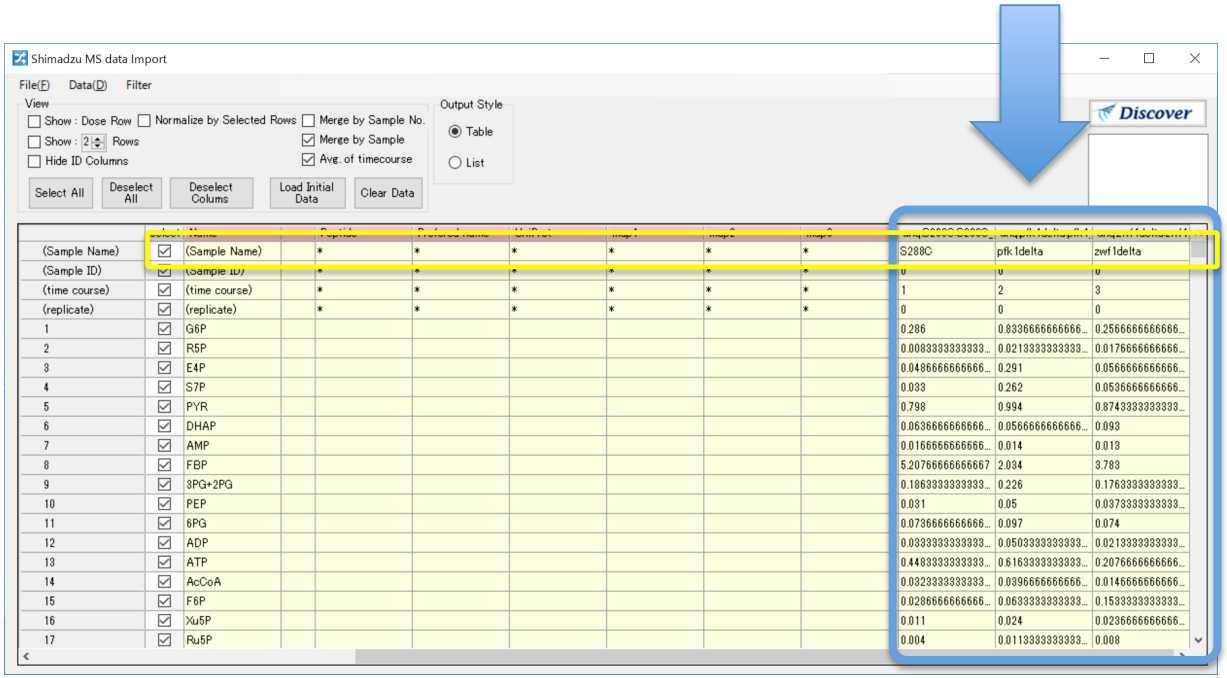
Shimadzu MSdata Import

Data Processing

- Clear Load Data
- Edit Data
- Imputate 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.



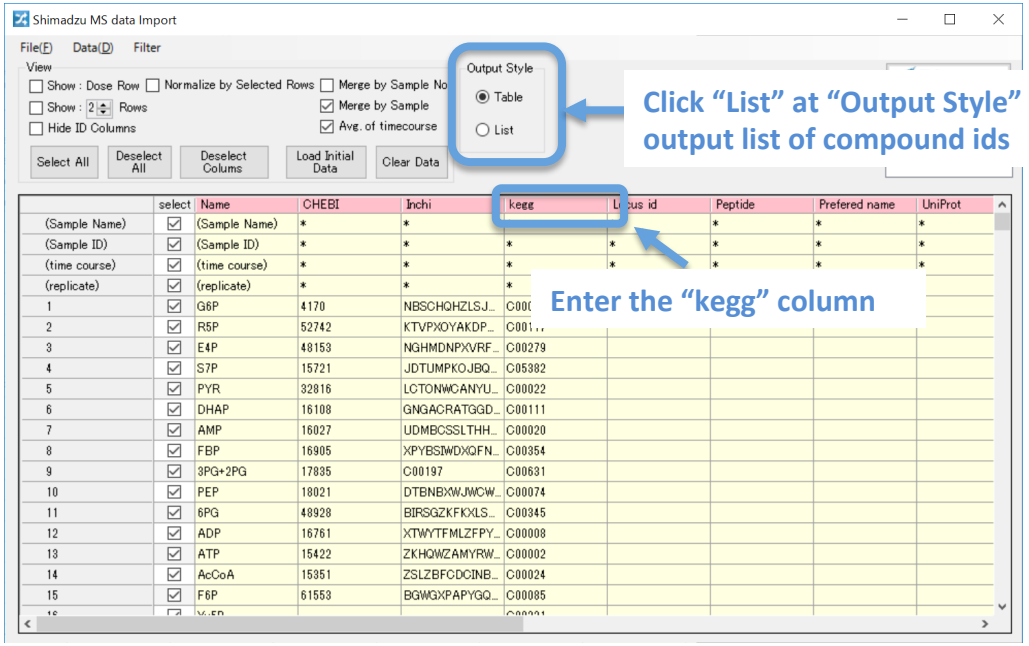


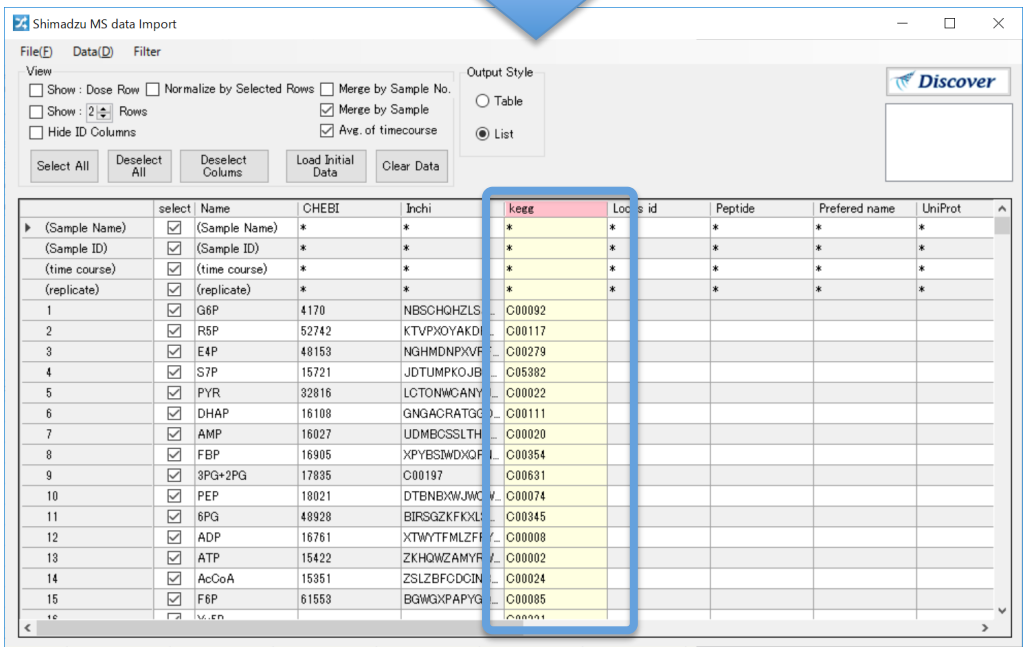
Shimadzu MSdata Import

Data Processing

- Clear Load Data
- Edit Data
- Imputate 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.





Shimadzu MSdata Import

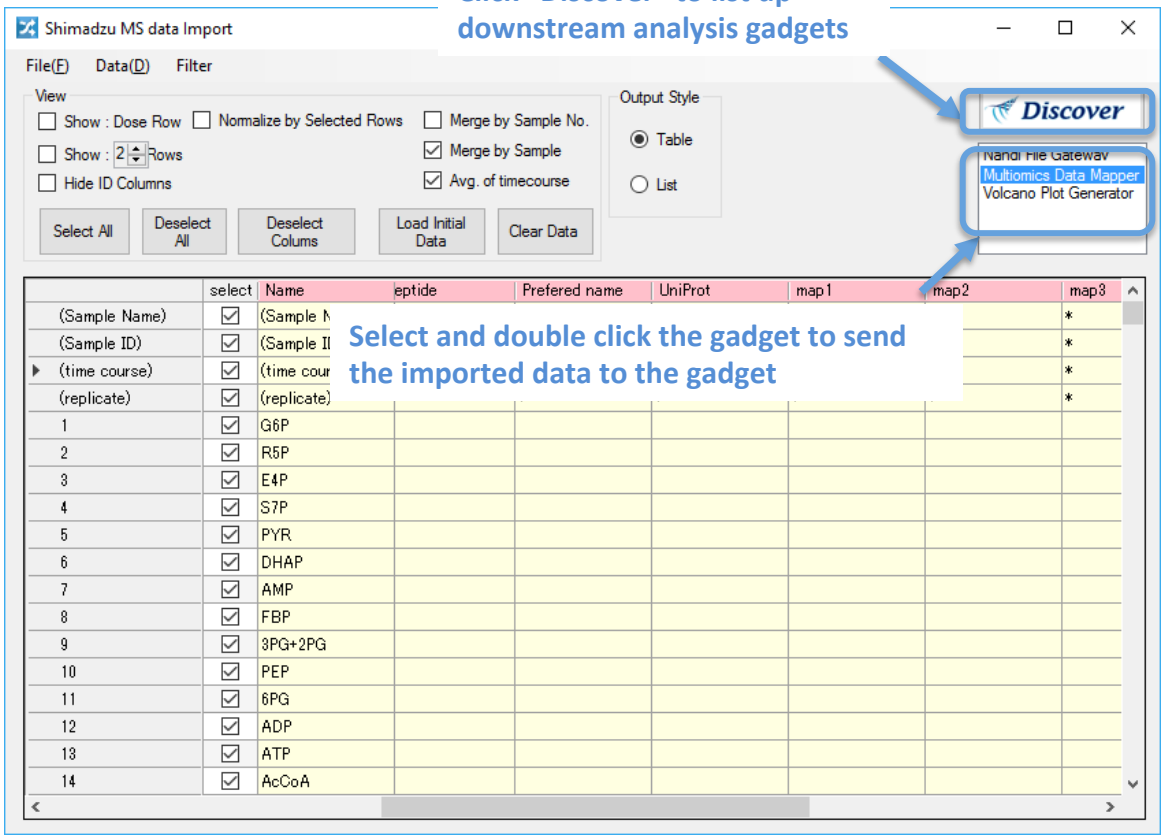
OUTPUT

- 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.



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

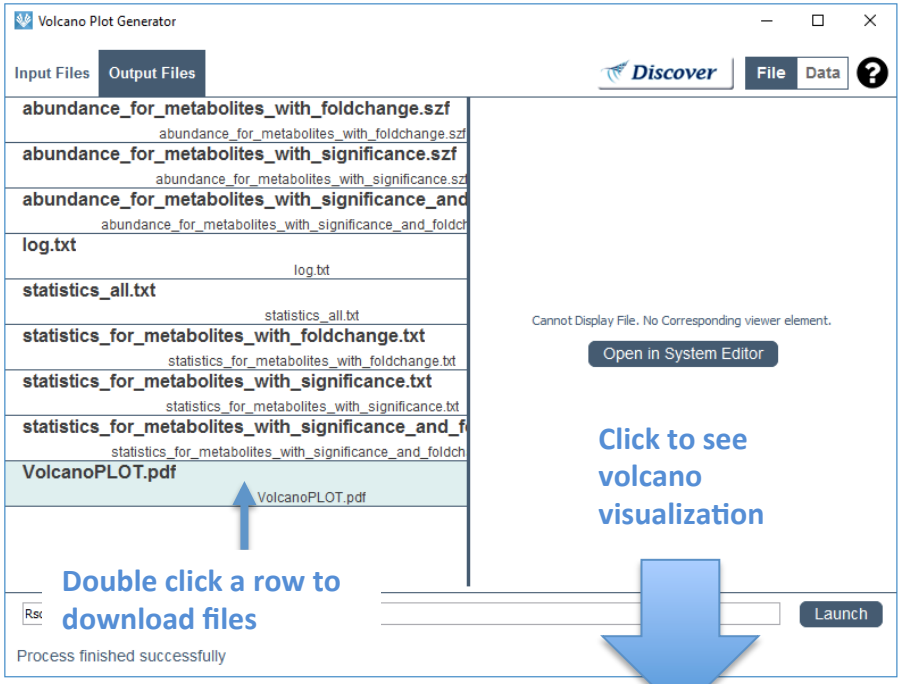
(.csv)

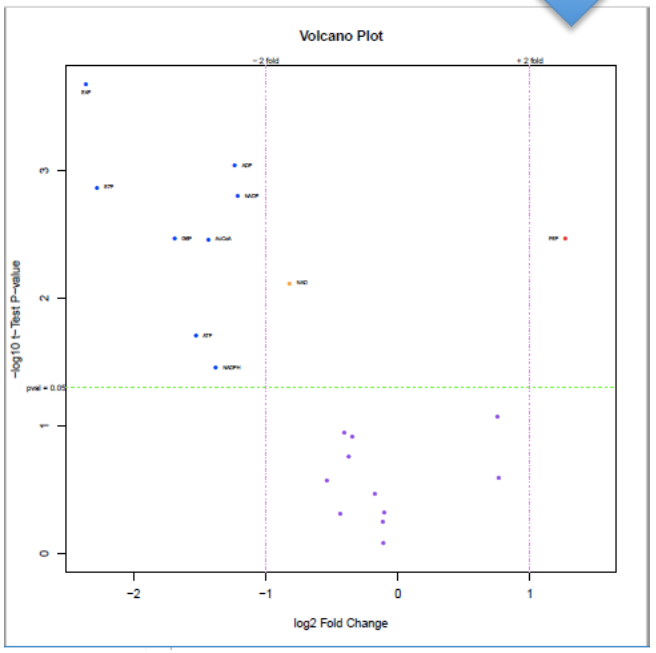
- **Volcano Plot Generator analysis for metabolome abundance**

OUTPUT

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

(.szf)





Volcano Plot Generator

INPUT

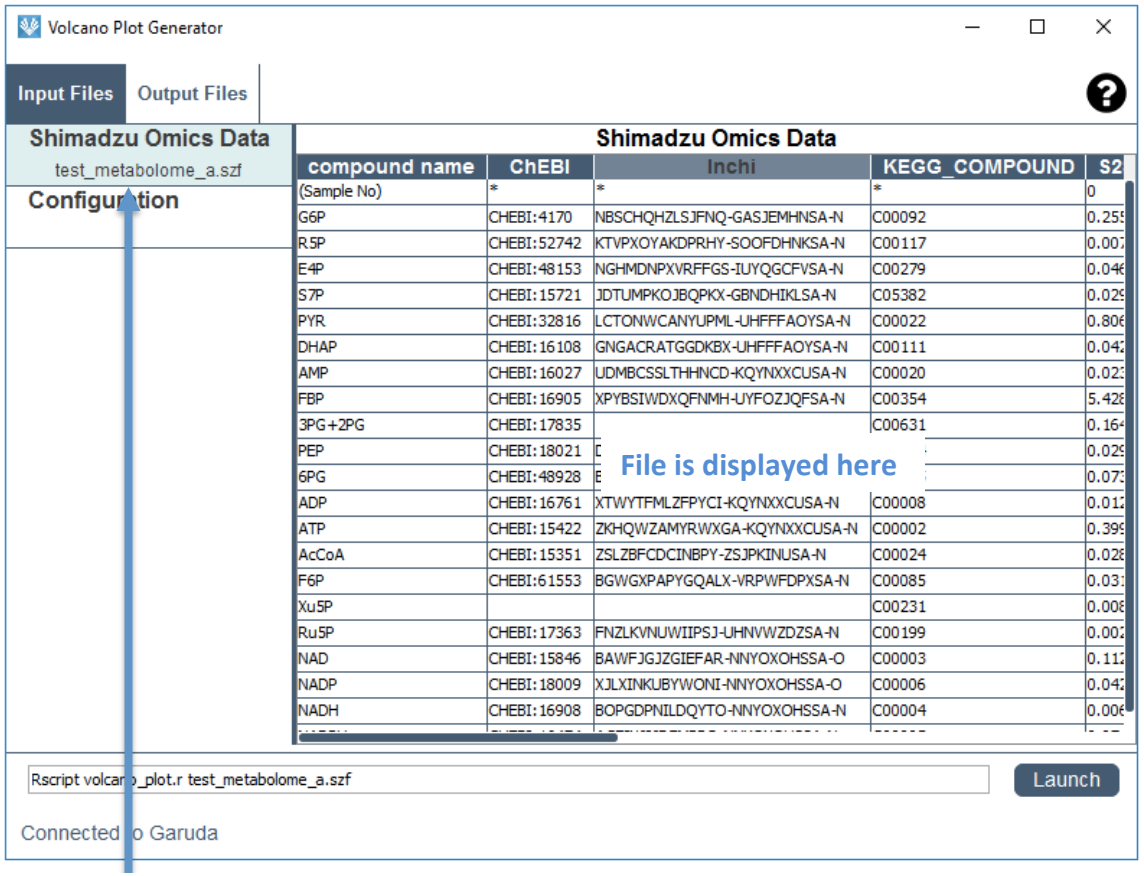
- Metabolite data

(.csv)

The gadget require 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 install the packages in your computer, if the gadgets were not installed in your computer.



Double click a rows to load files

Volcano Plot Generator

[parameter settings]

1. **Click “Configuration” on the left panel.**

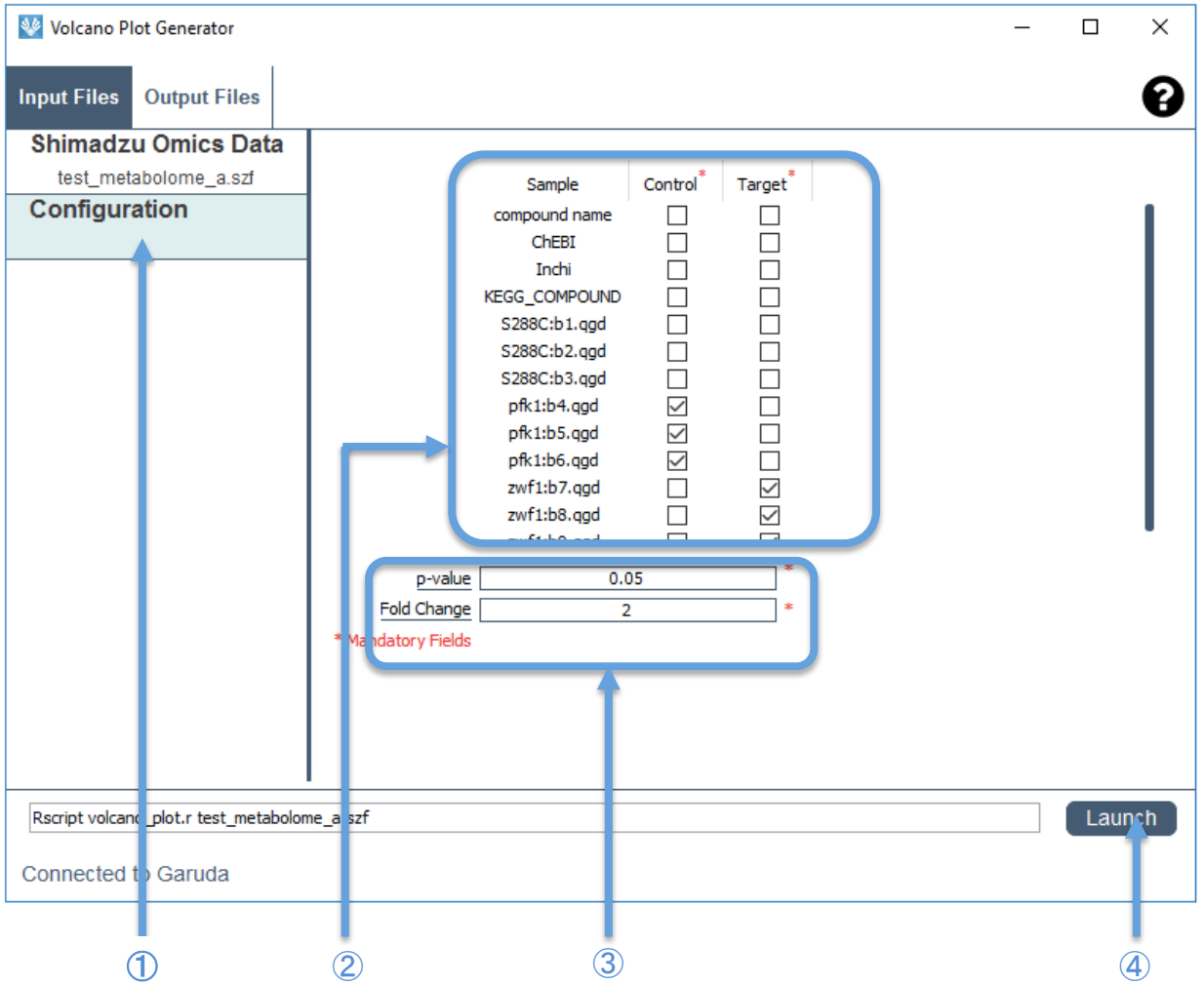
2. **Select “Control” and “Target” samples for Volcano Plot Generator analysis.**

   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



Volcano Plot Generator

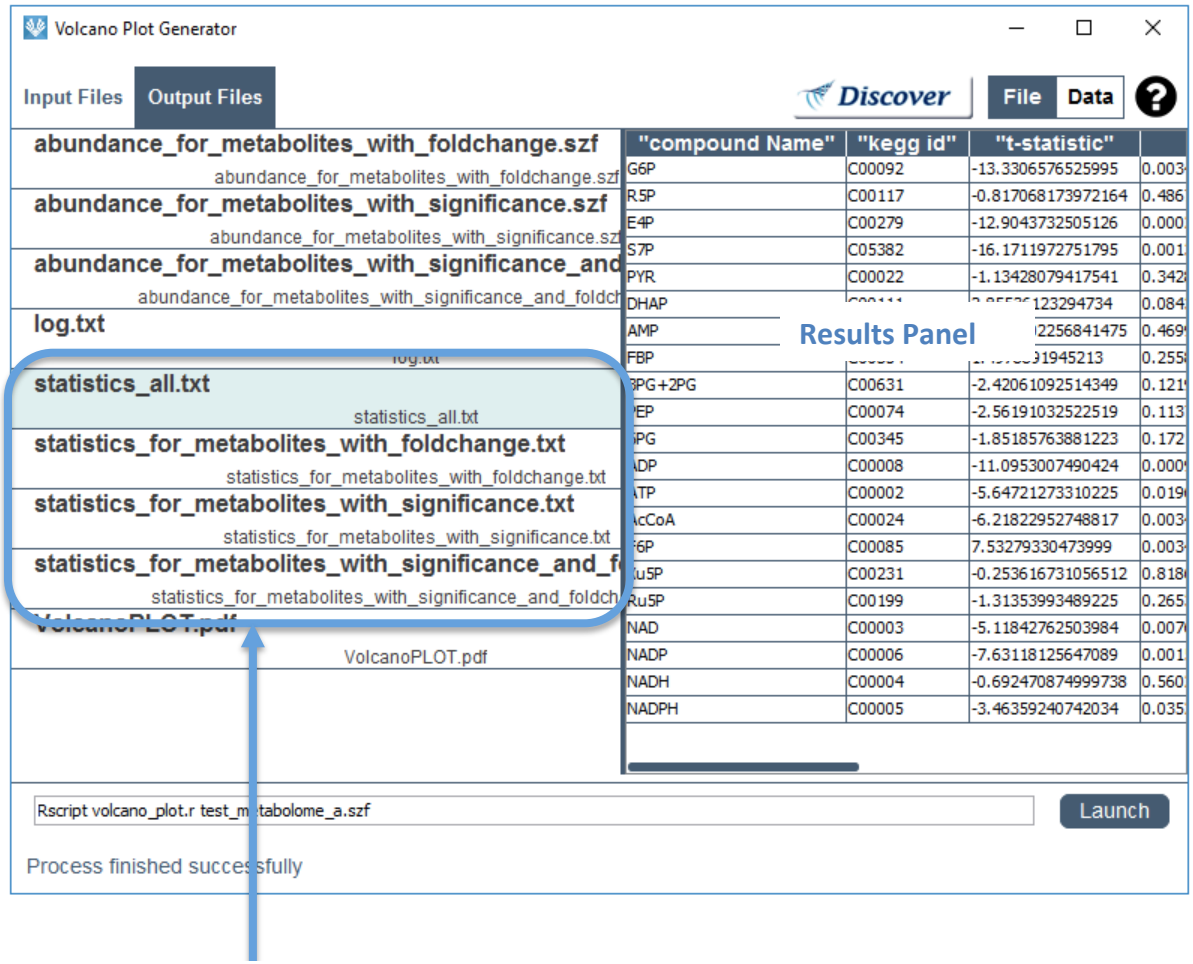
OUTPUT

- **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.



Double click a row to download files

Volcano Plot Generator

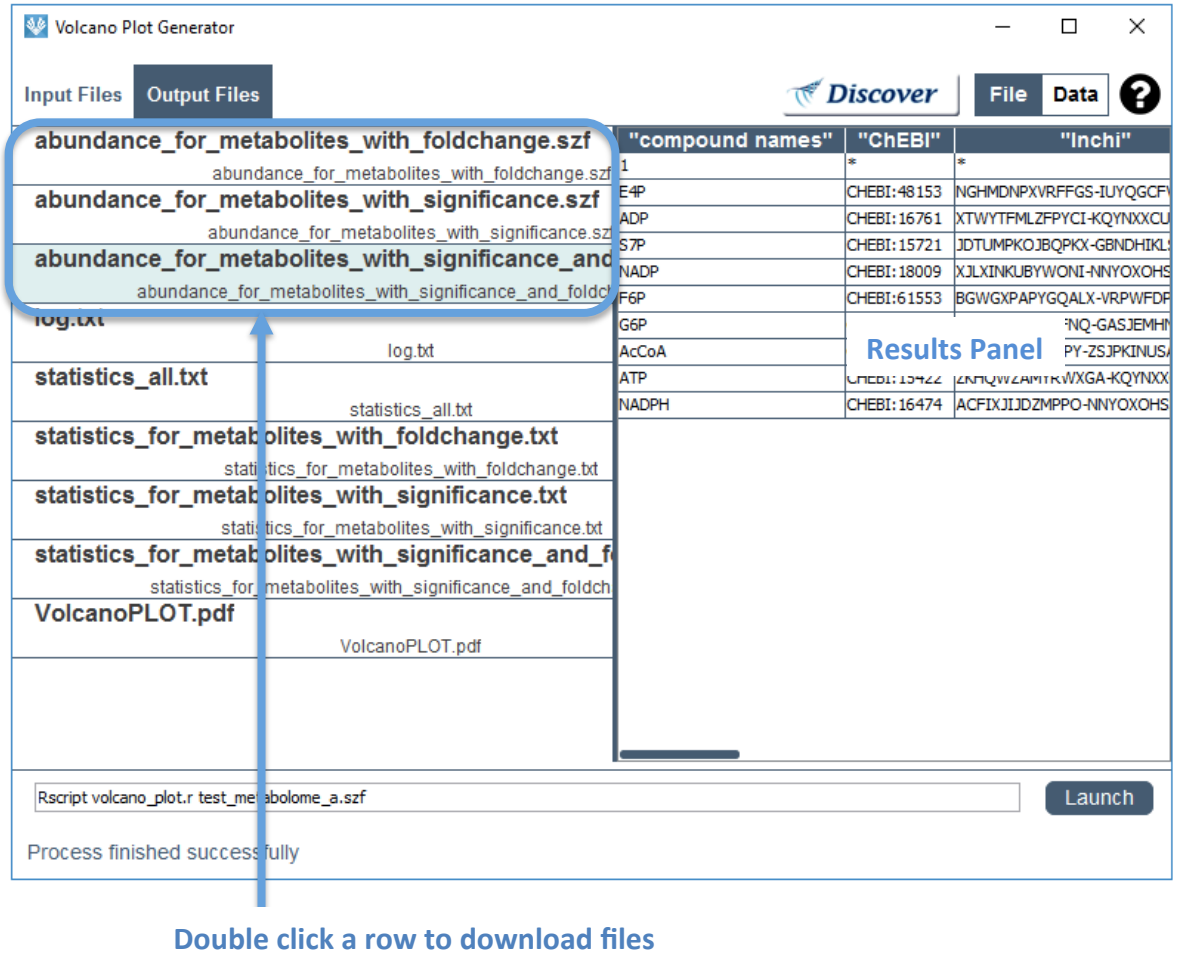
OUTPUT

- 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.



Double click a row to download files

Volcano Plot Generator

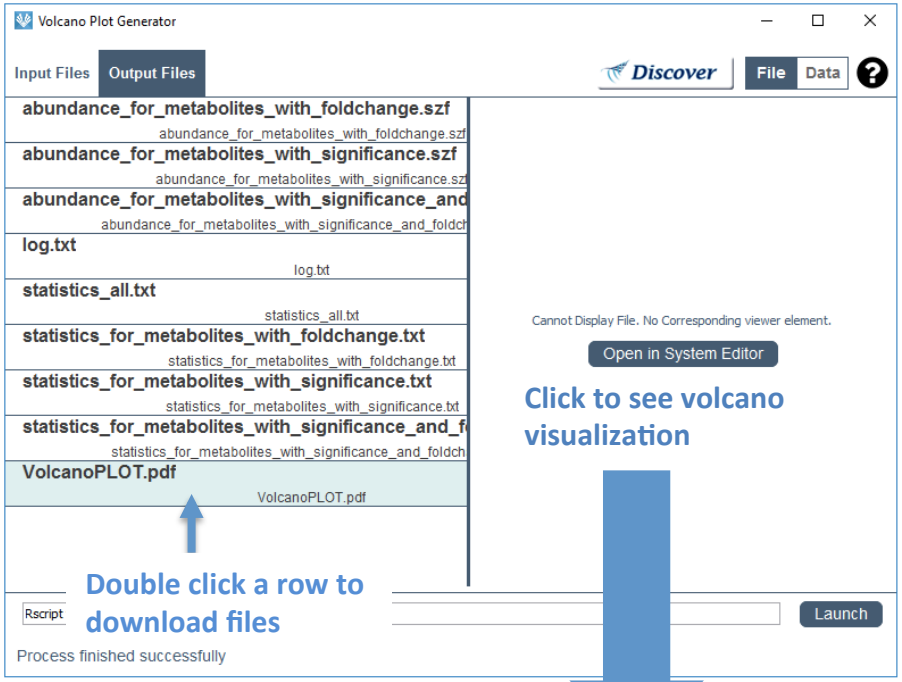
OUTPUT

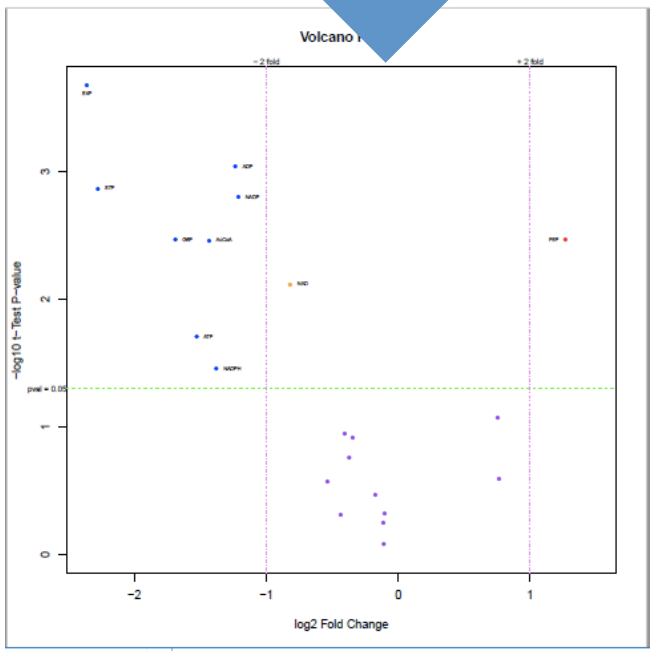
- Statistics from Volcano Plot Generator analysis
- Metabolome abundance data from Volcano Plot Generator analysis.
- **Volcano Plot Generator visualization (.szf)**

Volcano Plot Generator visualization

1. **Click on the right panel to display volcano visualization.**

2. **Double click the row "VolcanoPLOT.pdf" to download files.**





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

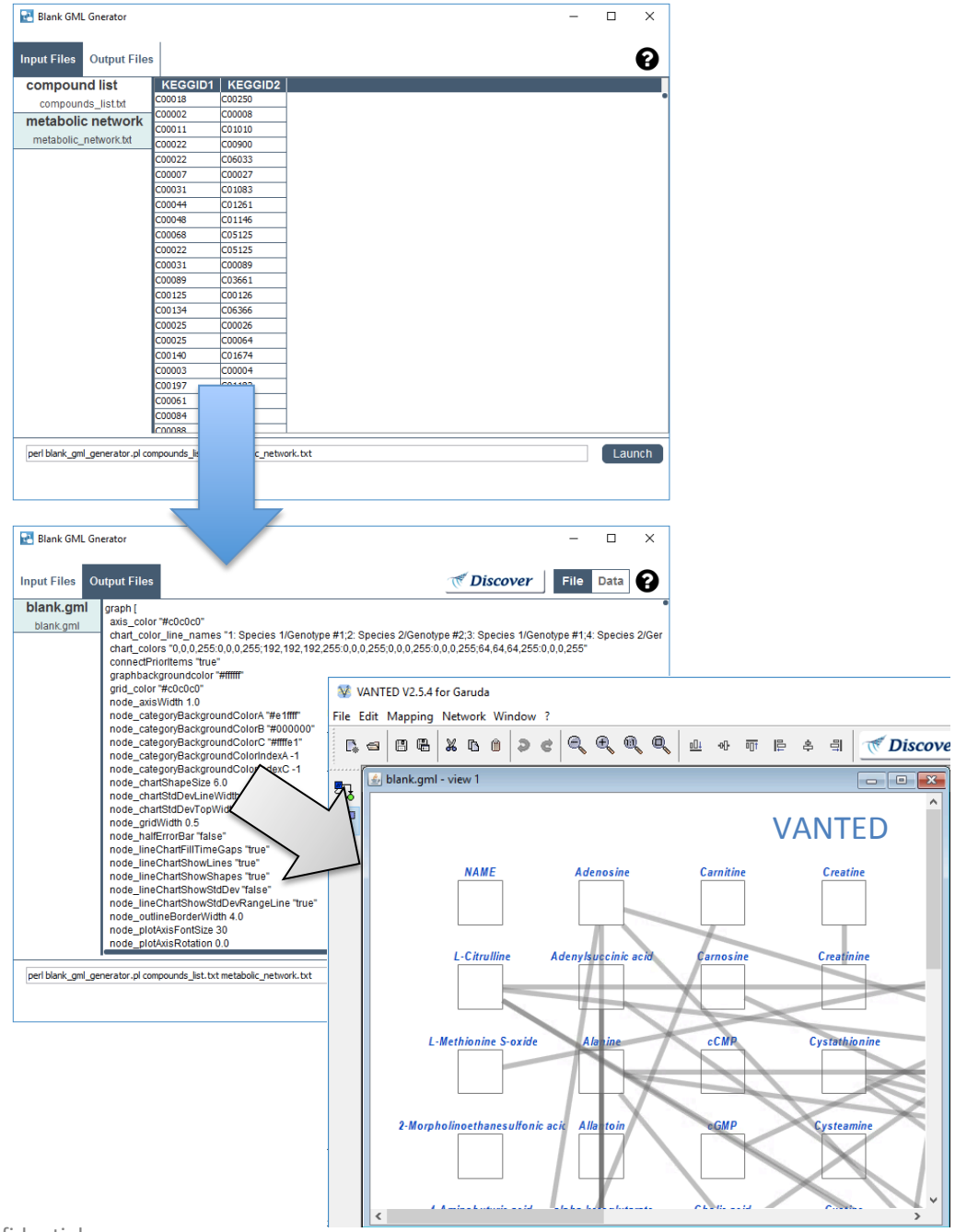
(.csv)

- **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

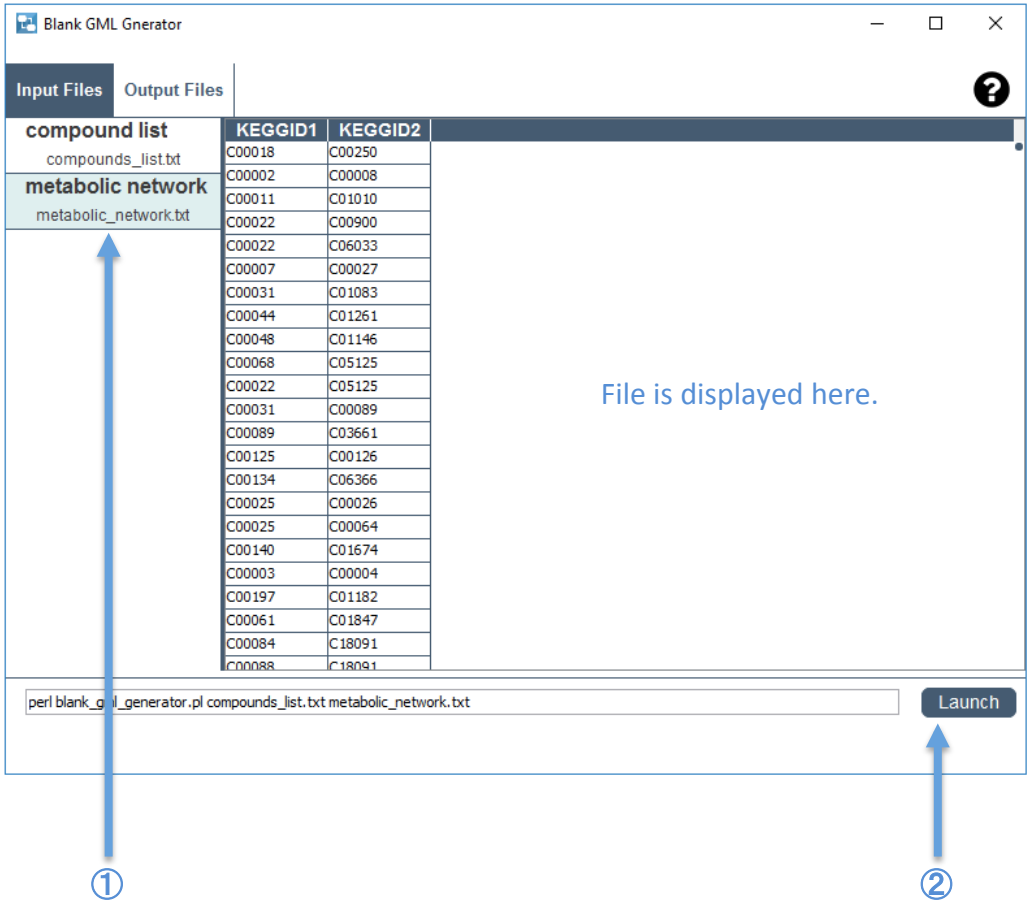
(.csv)

The gadget require 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 rows to load files
2. Click the "**Launch**" bottom to make blank .gml file after data upload



Sample File:
Sample file to test is available under **ShimadzuGadgets_SampleData> BlankGMLGenerator**

Blank GML Generator

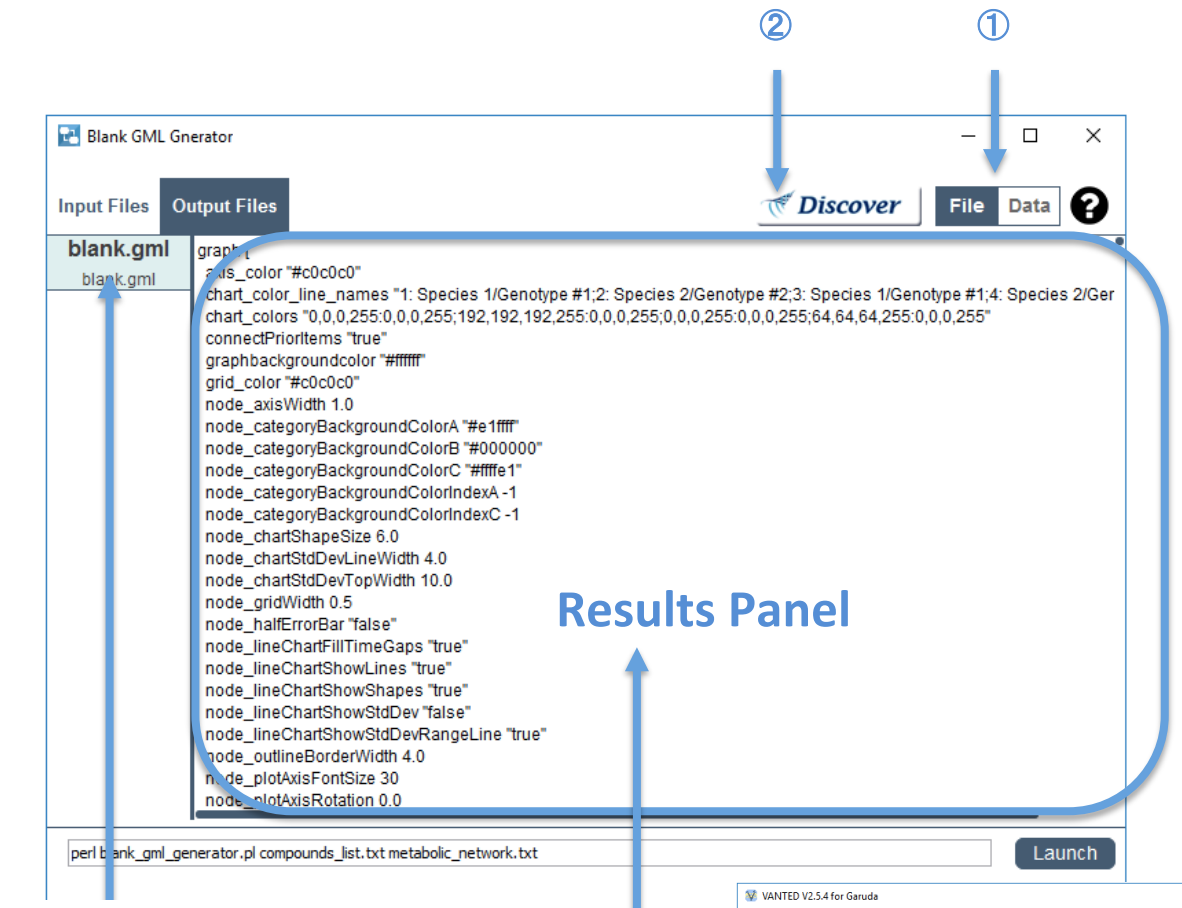
OUTPUT

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

(.gml)

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

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



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

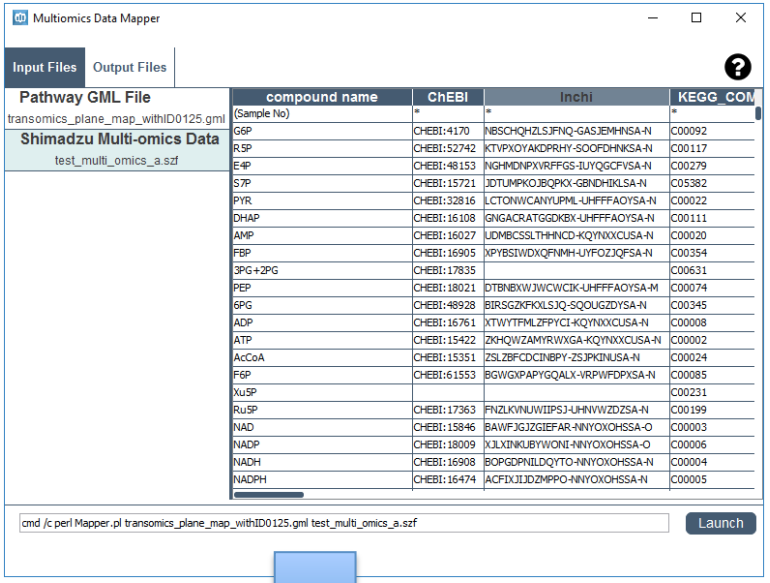
(.gml)

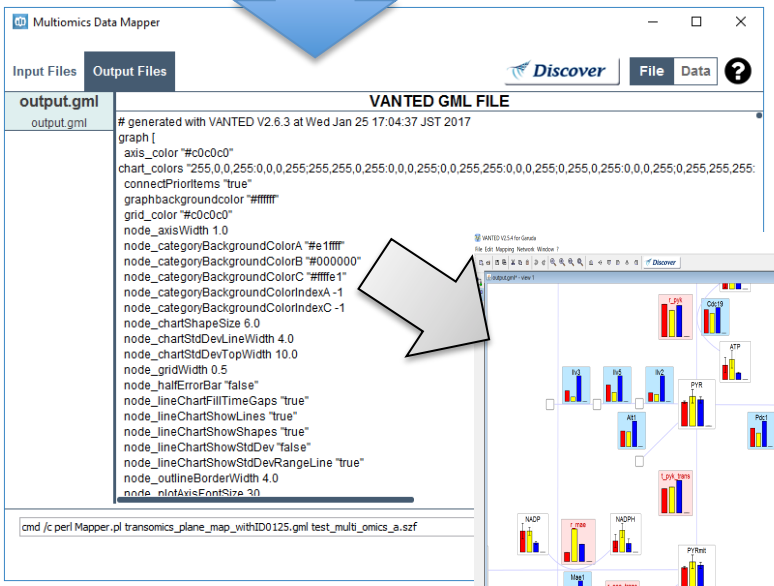
- **Merge Shimadzu multi-omics data with GML file for VANTED**

OUTPUT

- Send data to VANTED

(.gml)





Multiomics Data Mapper

INPUT

- Merged .szf data output from Shimadzu MSdata Import

(.szf)

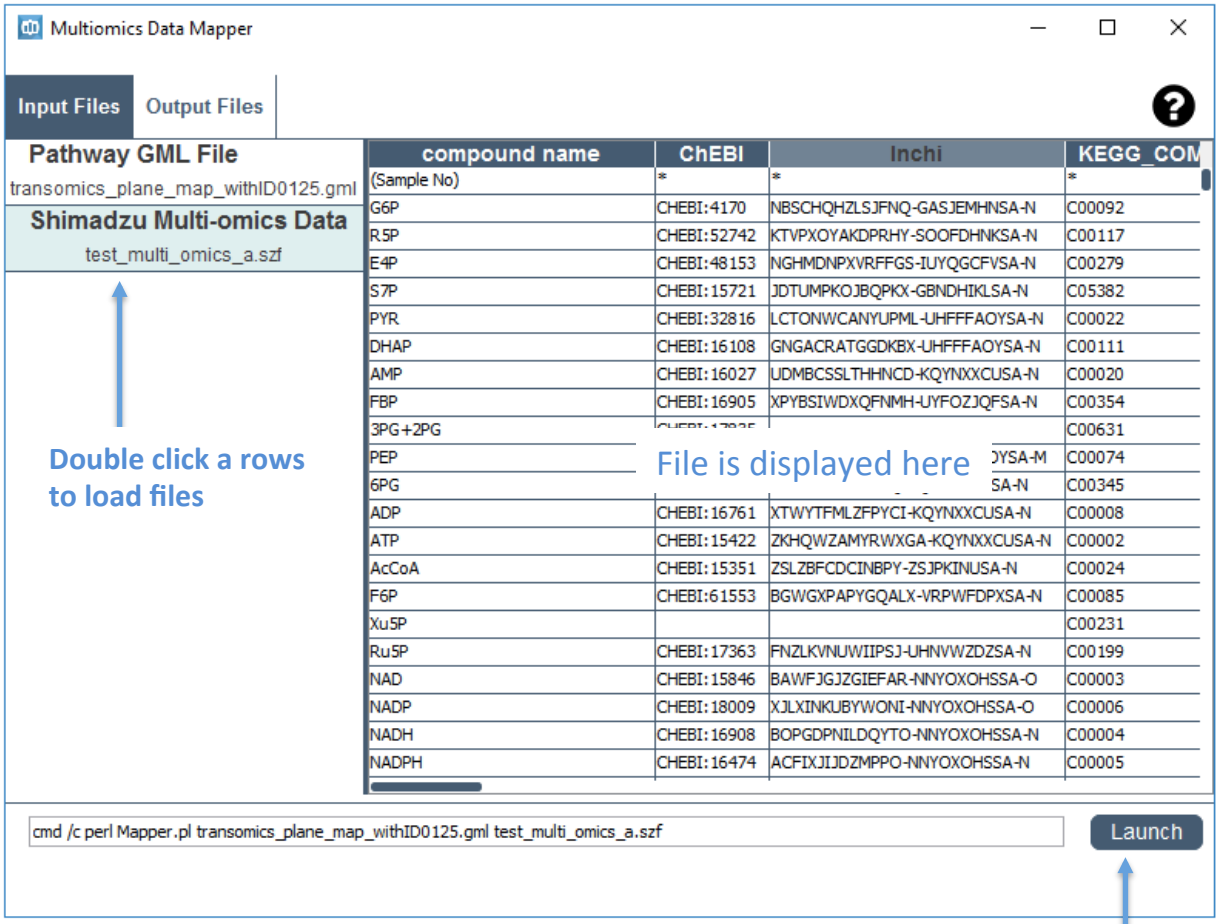
- .gml file for VANTED

(.gml)

The gadget require two input files;
(1) glm file for blank metabolic pathway map
(e.g., transomics_plane_map_withID0125.gml)
(2) 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

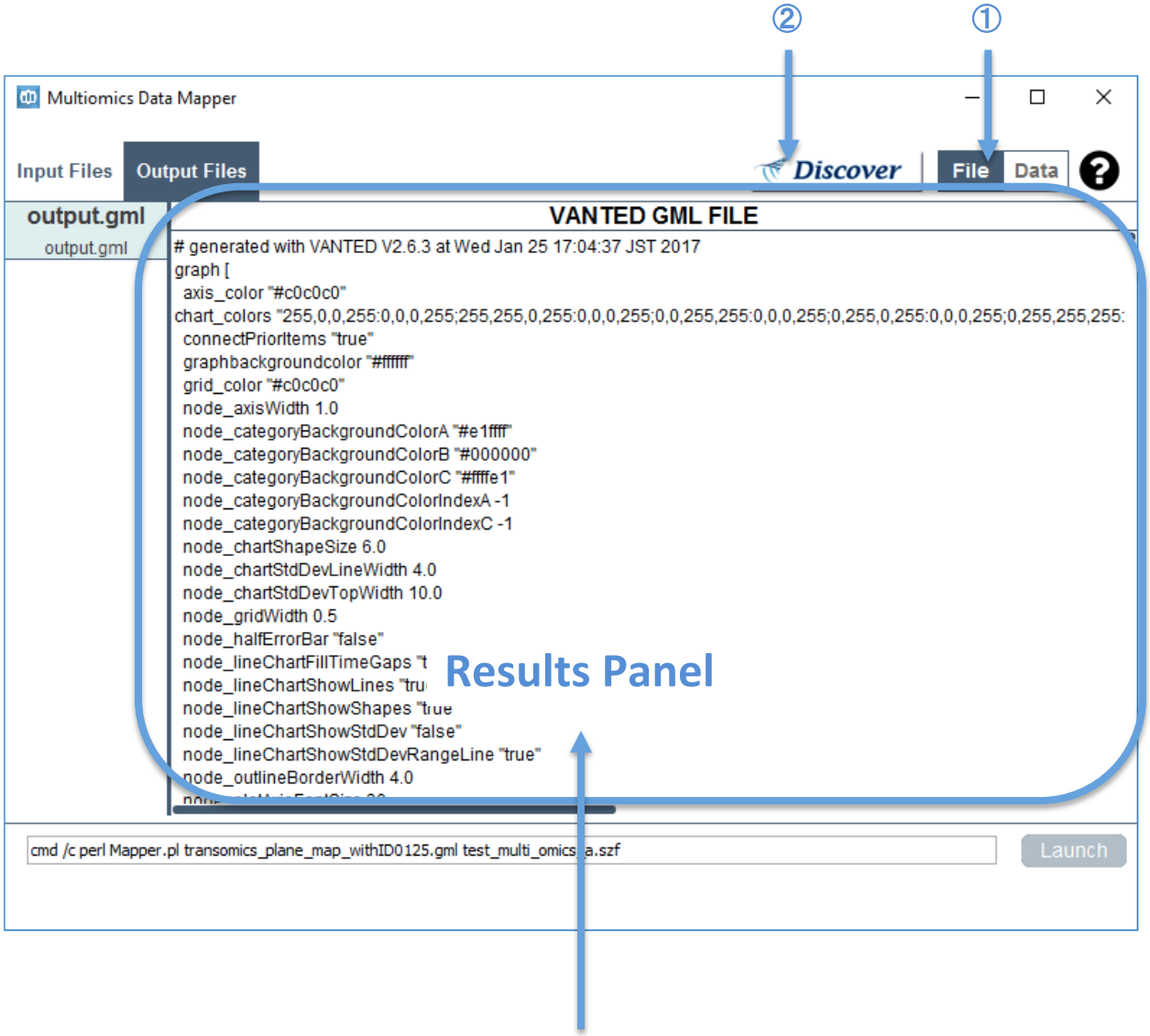
OUTPUT

- Send data to VANTED

(.gml)

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

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



Resultant merged gml is shown in the result panel

Garuda Recipes

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

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.

INPUT

- .gml file from "Multiomics Data Mapper" gadget

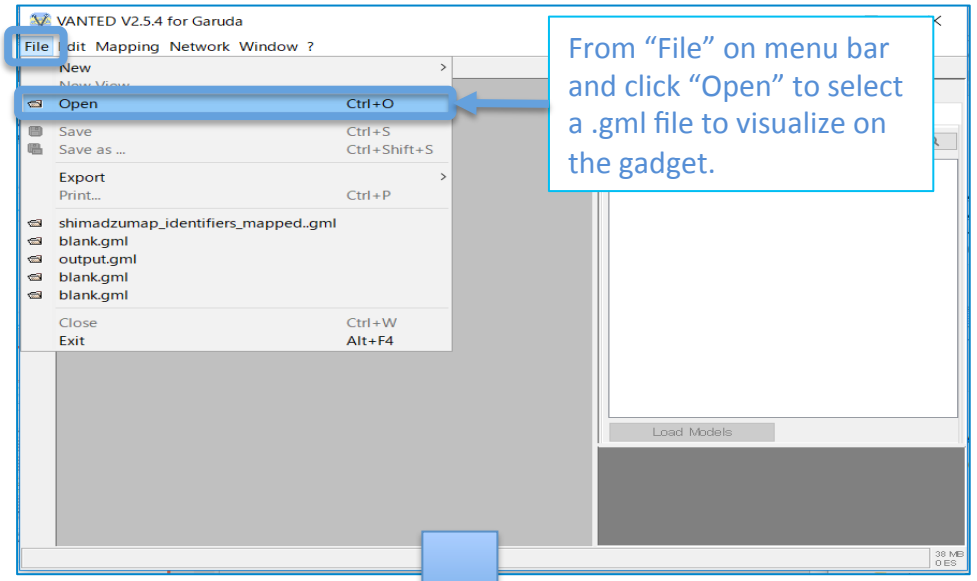
(.GML)

- **Visualize multiomics data over VANTED pathway map.**

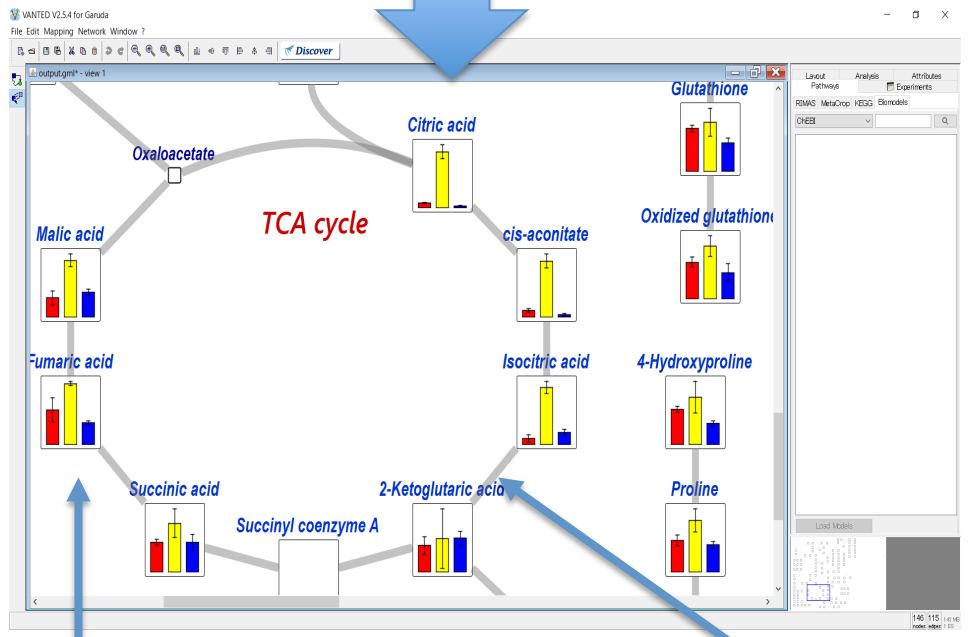
OUTPUT

- Image file

(.png)



From "File" on menu bar and click "Open" to select a .gml file to visualize on the gadget.



Metabolome abundance data of a metabolite are visualized as bar graph below the name of the metabolite.

Reactions

iPATH2

This gadget maps and visualizes KEGG ids on KEGG pathway maps

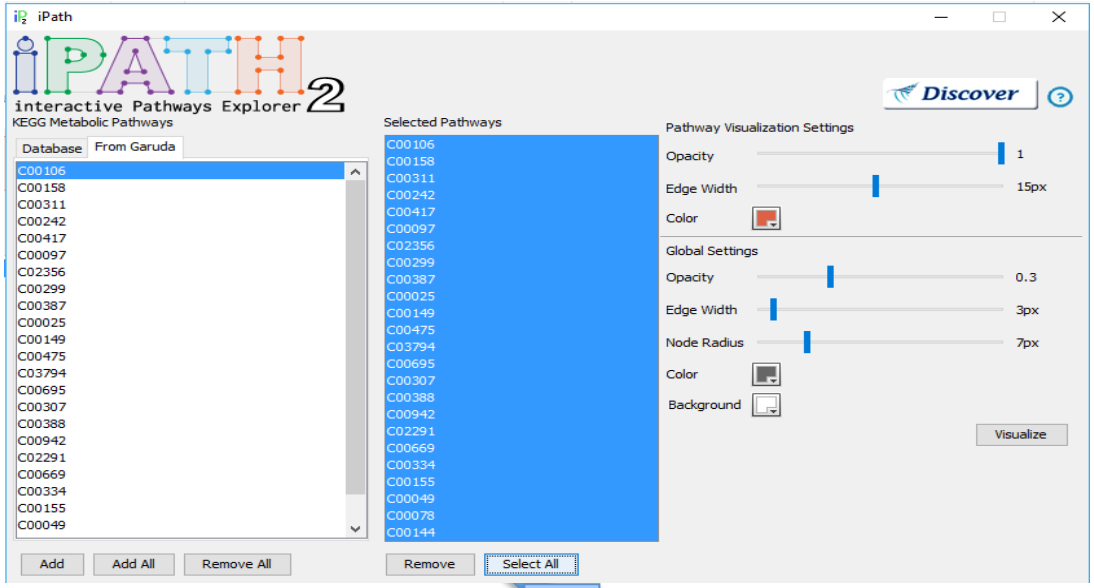
INPUT
- KEGG IDs

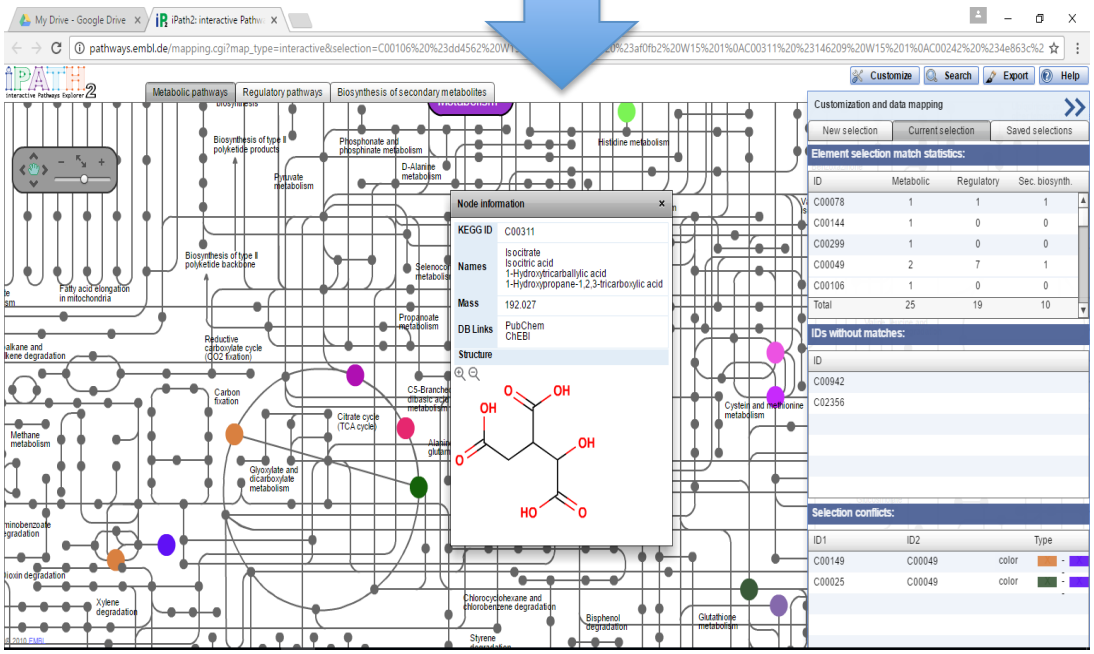
(.szf / .txt)

- **Visualize KEGG ids on KEGG pathway maps**

OUTPUT
- Image file

(.png)



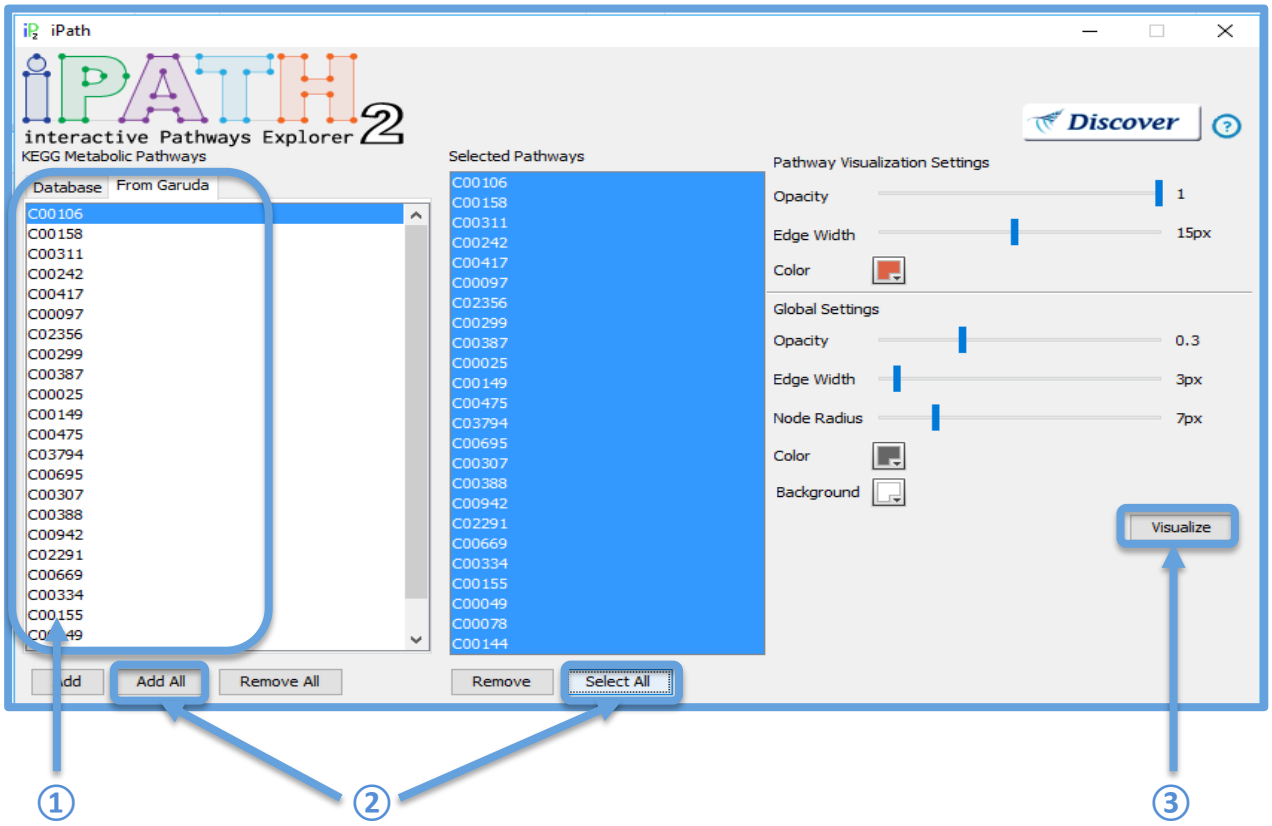


iPATH2

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.

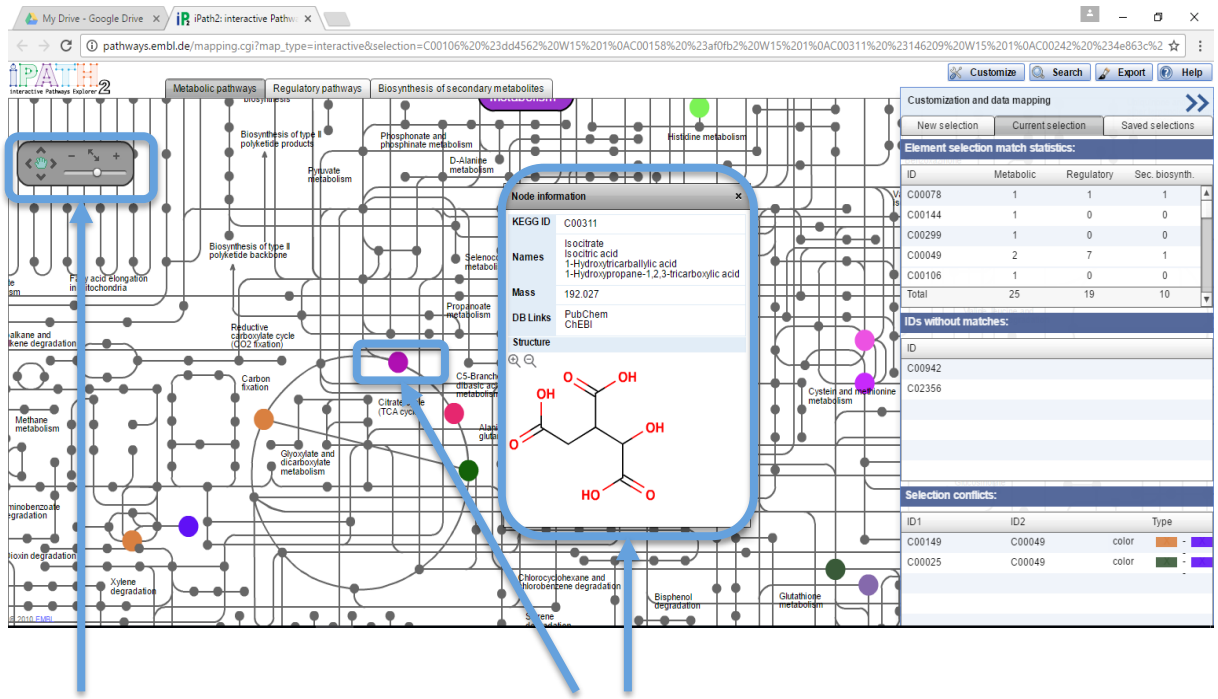


iPATH2

This gadget maps and visualizes KEGG ids on KEGG pathway maps

[Visualize]

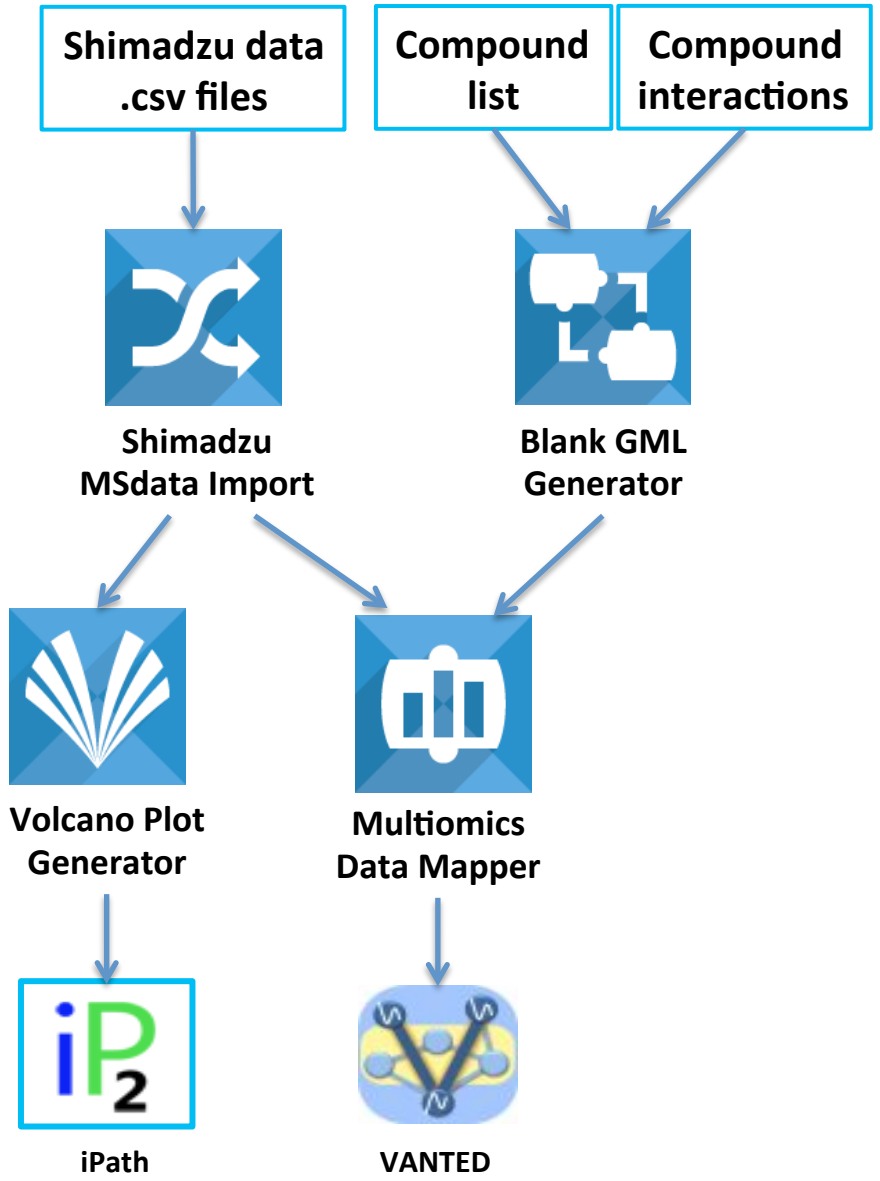
- Click to **zoom up/down** the map and to **explore** the map.
- **Selected metabolites** are enlarged and colored on the map. Click to see details about the metabolites.



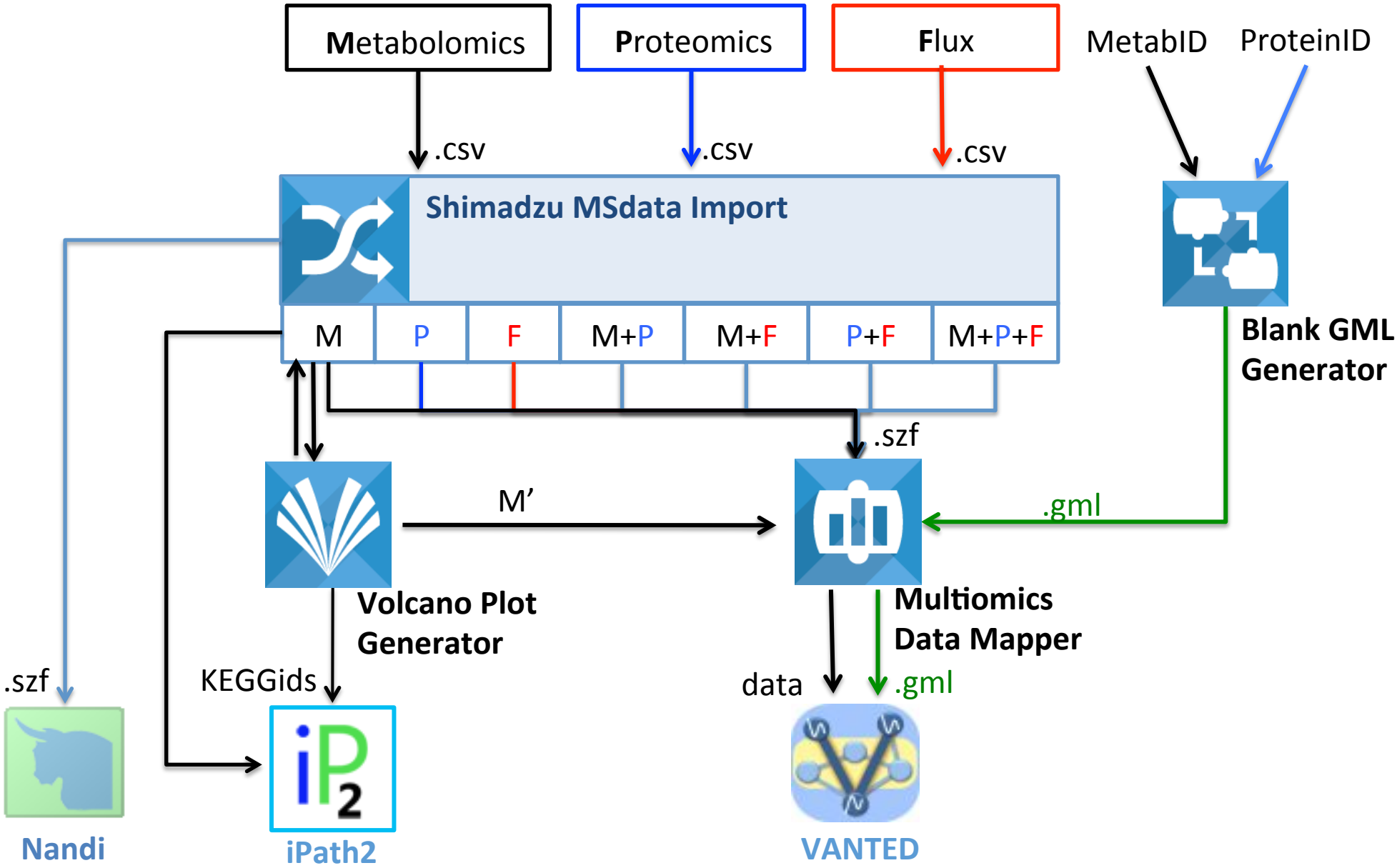
Click to zoom up/down the map and to explore the map.

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

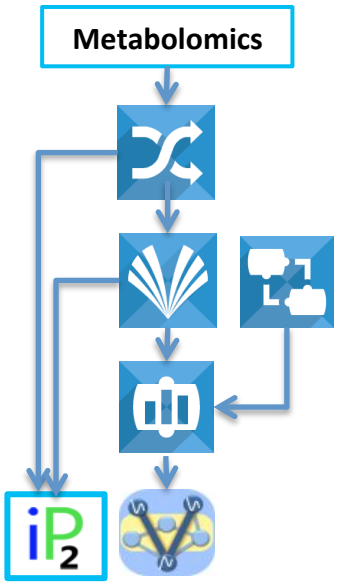
Multiomics Data Analysis Recipes Examples



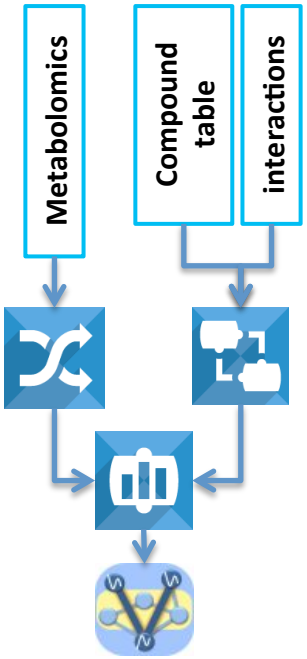
Connectivity among gadgets for potential recipes



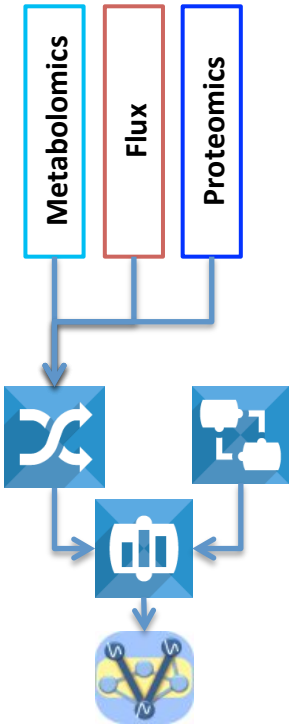
Recipe #1 :
Visualize
Metabolite Data to
Metabolomic Pathway



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

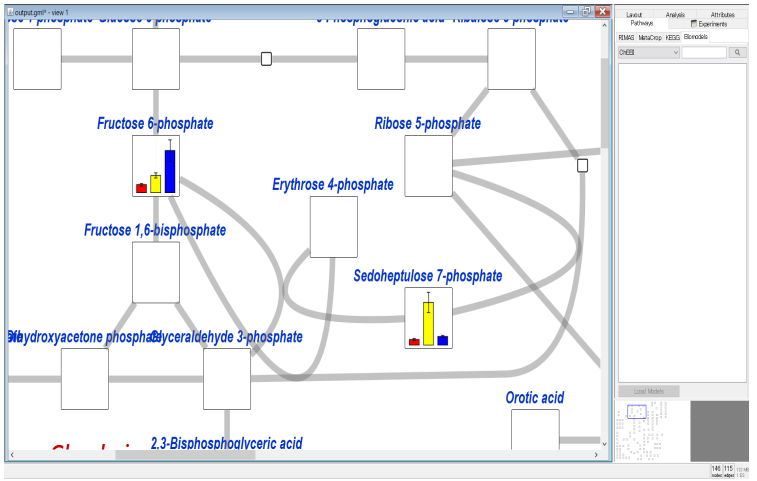
The recipe conducts **Volcano Plot Generator analysis to identify significant metabolites**.
Then abundance of the significant metabolites are **mapped on the metabolic network** through "**iPath**" or "**Vanted**"

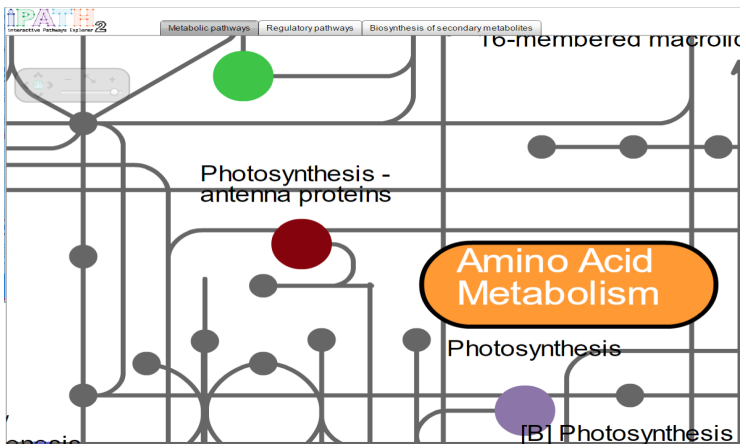
Input

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

Gadgets for Cooking Data

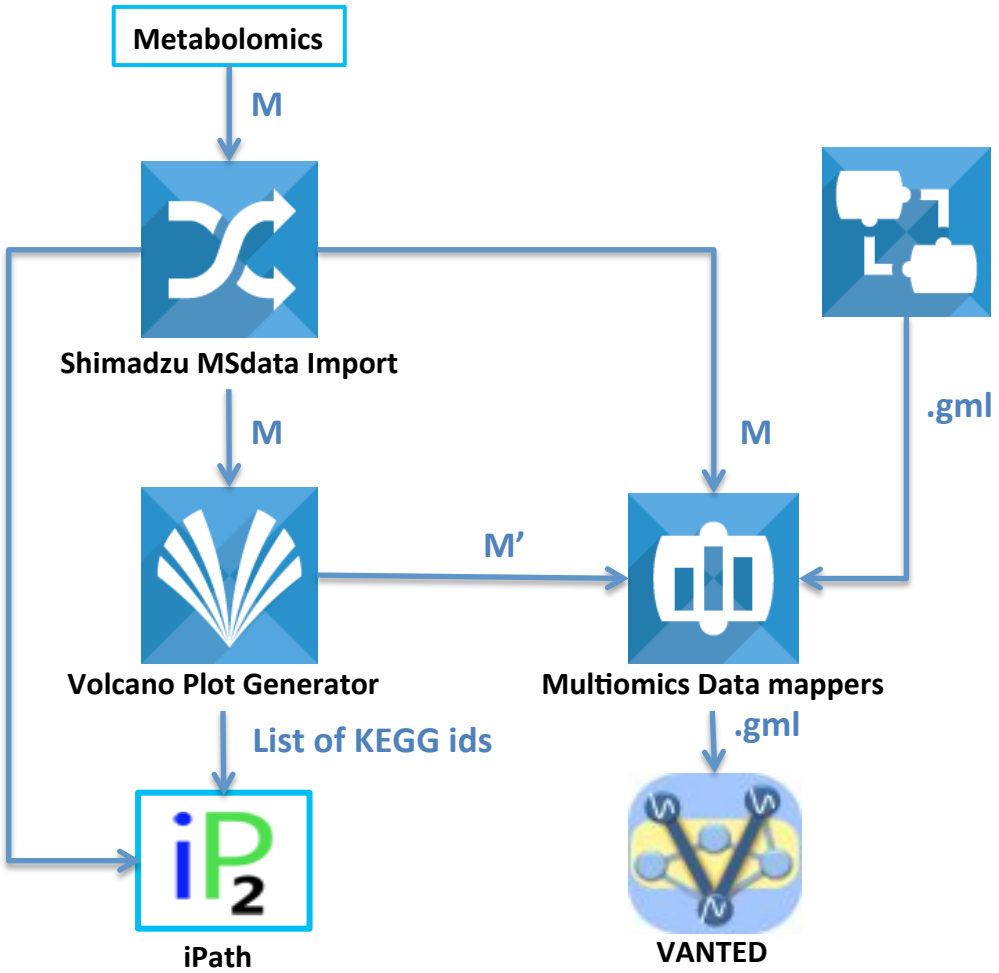
OUTPUT

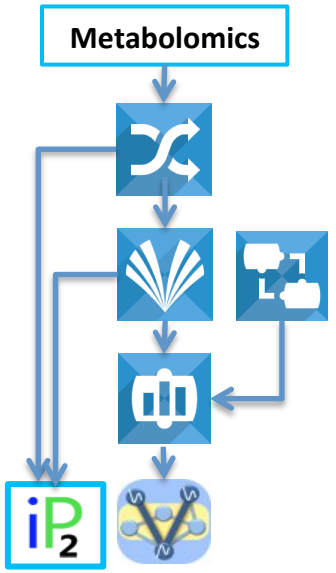




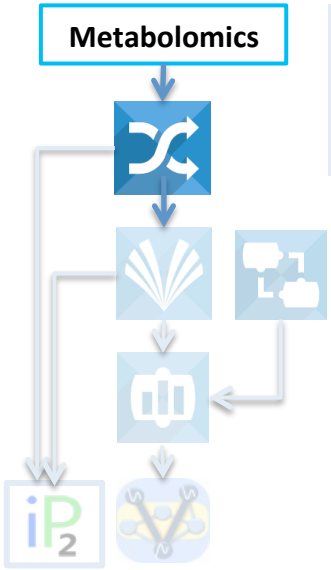
Recipe #1 : Visualize Metabolite Data to Metabolomic Pathway

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**"





Recipe #1 : Visualize Metabolite Data to Metabolomic Pathway

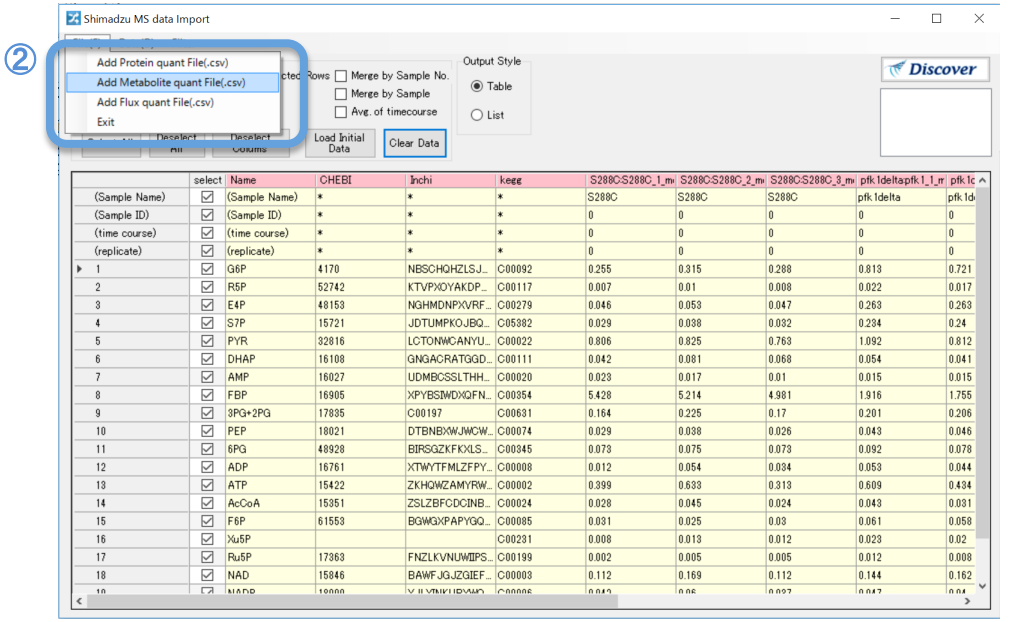


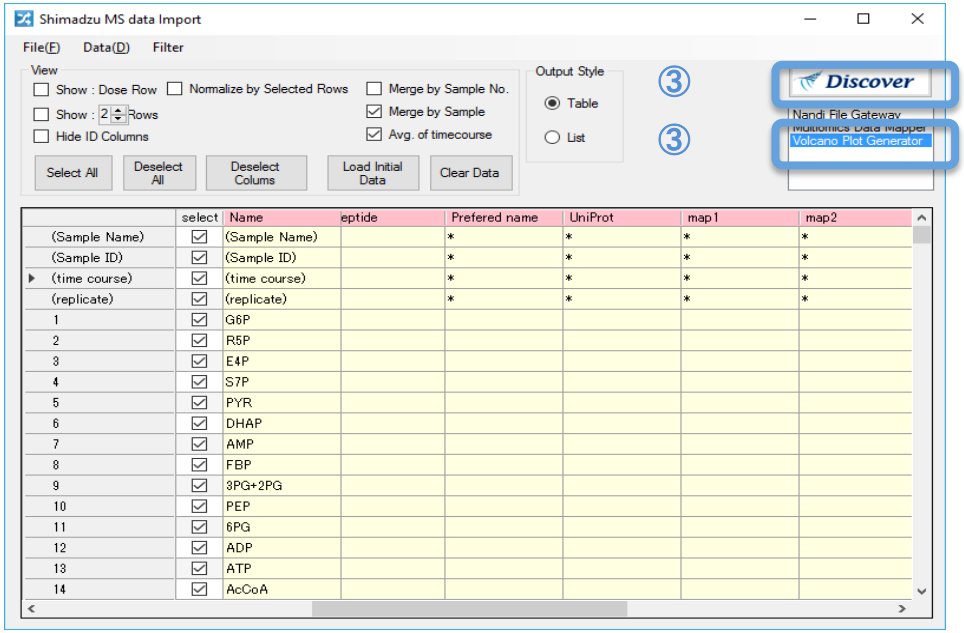
STEP 1. Format the Shimadzu metabolome abundance data for downstream analysis gadgets

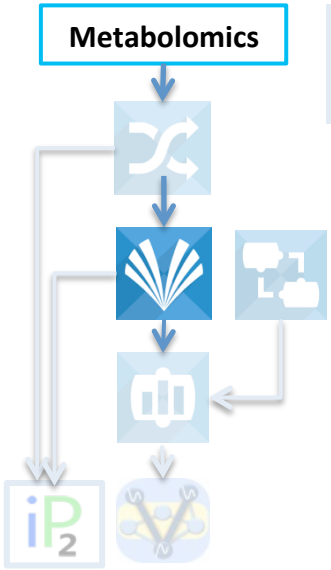
1. From the Garuda dashboard, select and double-click the **"Shimadzu MSdata Import"** gadget to launch the gadget.

2. 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).

3. 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.







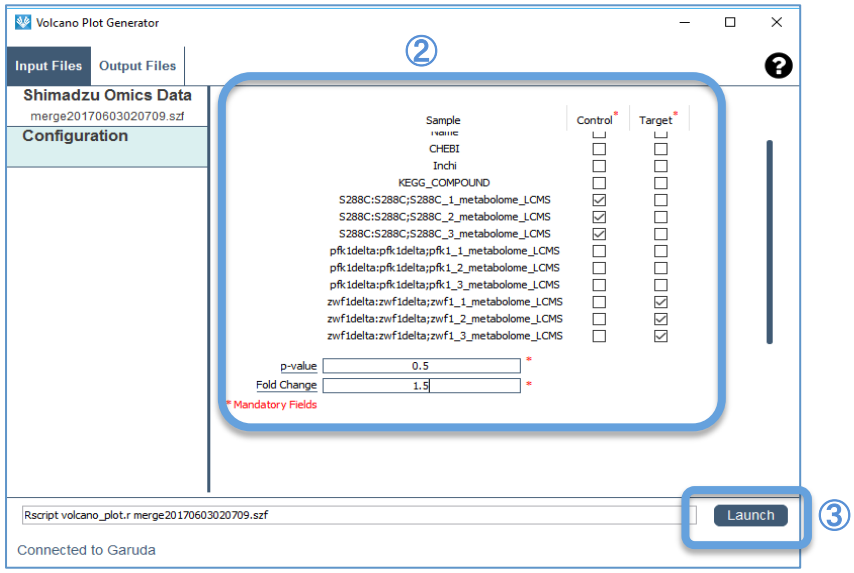
STEP 2. Volcano Plot Generator analysis for Shimadzu metabolome abundance

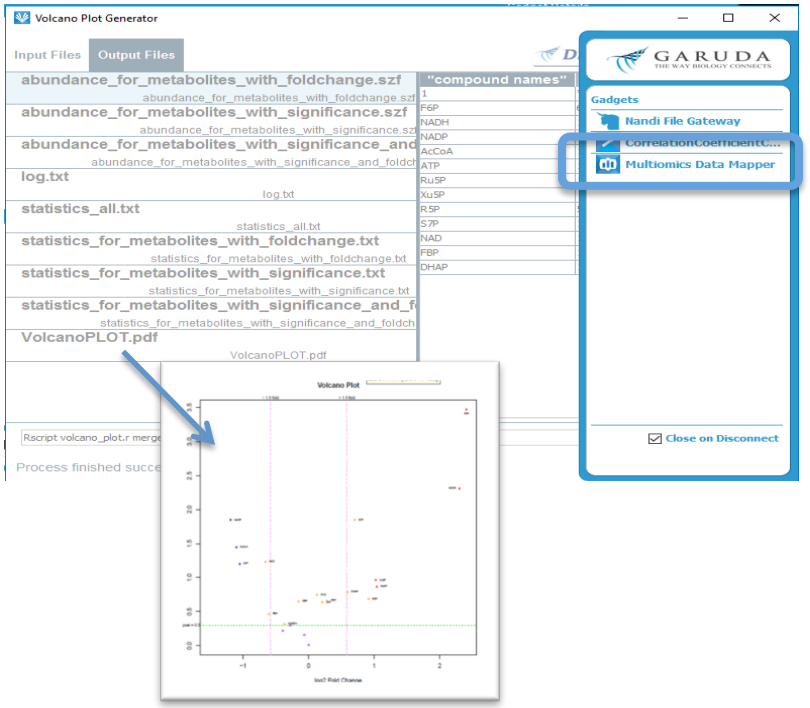
1. From "**Shimadzu MSdata Import**", select and double click "**Volcano Plot Generator**". Garuda will launch the gadget and send the formatted data to the gadget.

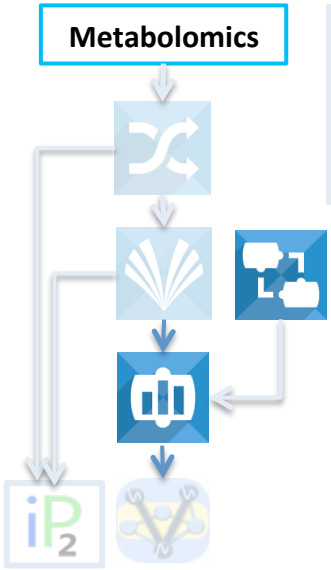
2. Set **parameters** (e.g., p-value and fold-change threshold as well as control and target samples). Please see help of "Volcano Plot Generator" gadget for details of the parameters.
(In this example, "S288C.b1.qgd, S288C.b2.qgd, S288C.b4.qgd" are "**Control**" samples, while "zwf1.b7.qgd, zwf1.b8.qgd, zwf1.b9.qgd" are "**Target**" samples.
P-value and Fol Change are 0.10 and 1.5, respectively).

3. Click "**Launch**" to do Volcano Plot Generator analysis.

4. 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 "**Multiomics Data Mapper**" to upload the data of abundance for significant metabolites to the Multiomics Data Mapper" gadget.







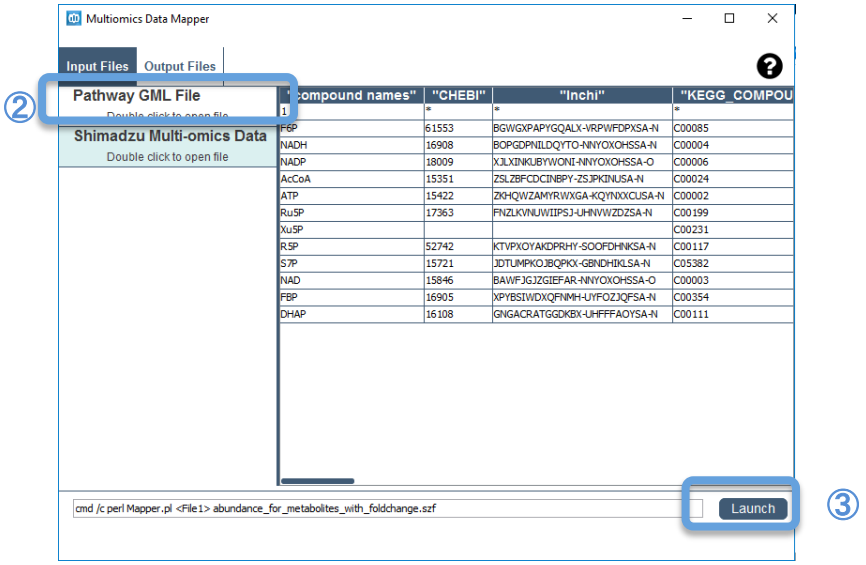
STEP 3 **Merge metabolome abundance data for significant metabolited from volcano analysis with gml file for blanck metabolic pathway**

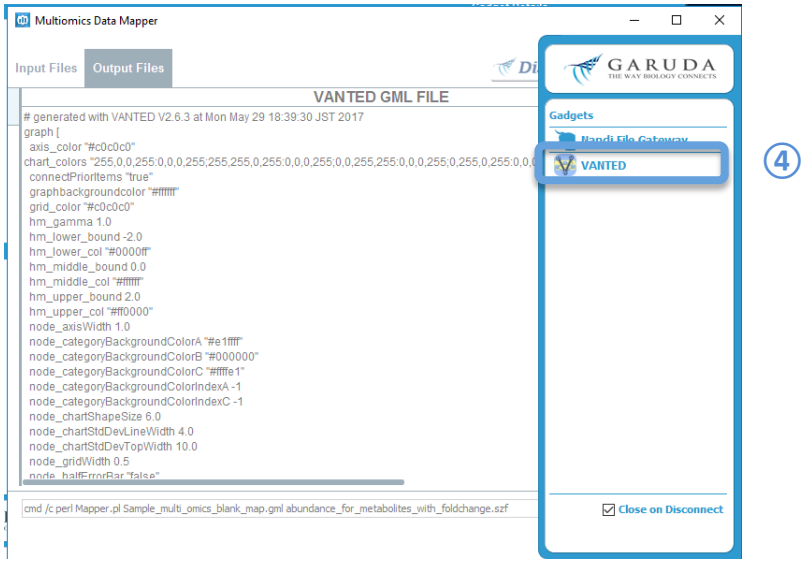
1. From "**Volcano Plot Generator**" discovery, select and double click "**Multiomics Data Mapper**".
   Garuda will launch the "Multiomics Data Mapper" gadget and send the metabolome data for identified metabolite by volcano analysis to the gadget

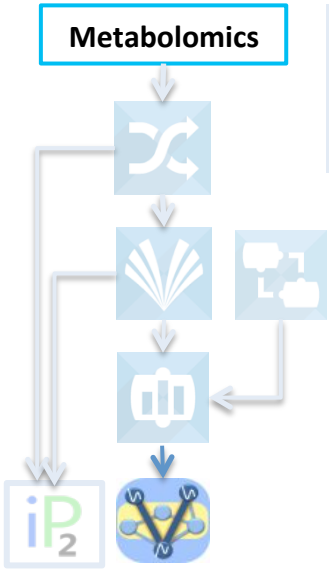
2. Click "**gml file**" to upload .gml file for blank metabolic network,
   "**Sample_multi_omics_blank_map**" (in ShimadzuGadgets_SampleData> MultiomicsDataMapper).

3. Click "**Launch**" to merge the formatted metabolome abundance data with blank metabolic network.

4. Select **File** and click **Discover**.
   You can find **VANTED** gadget.



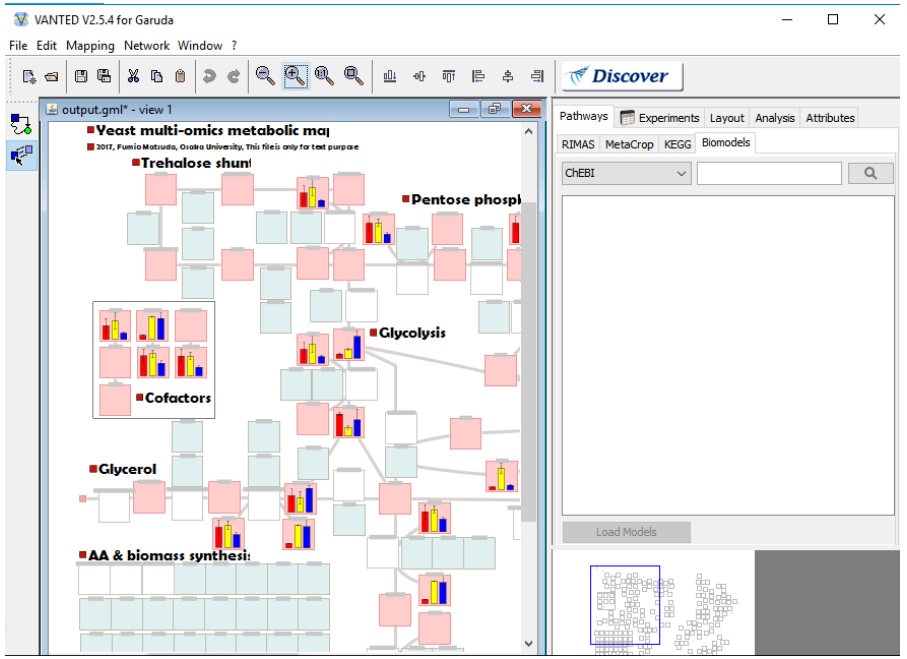


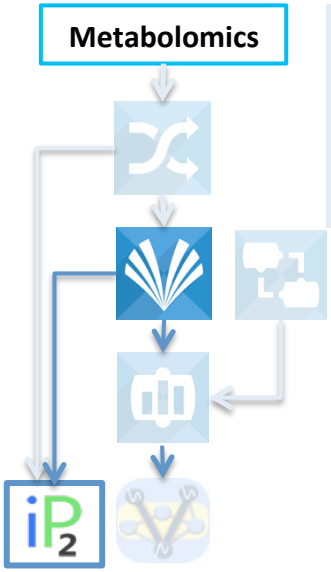


STEP 4. Visualize metabolome abundance data on metabolic network through VANTED.

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.





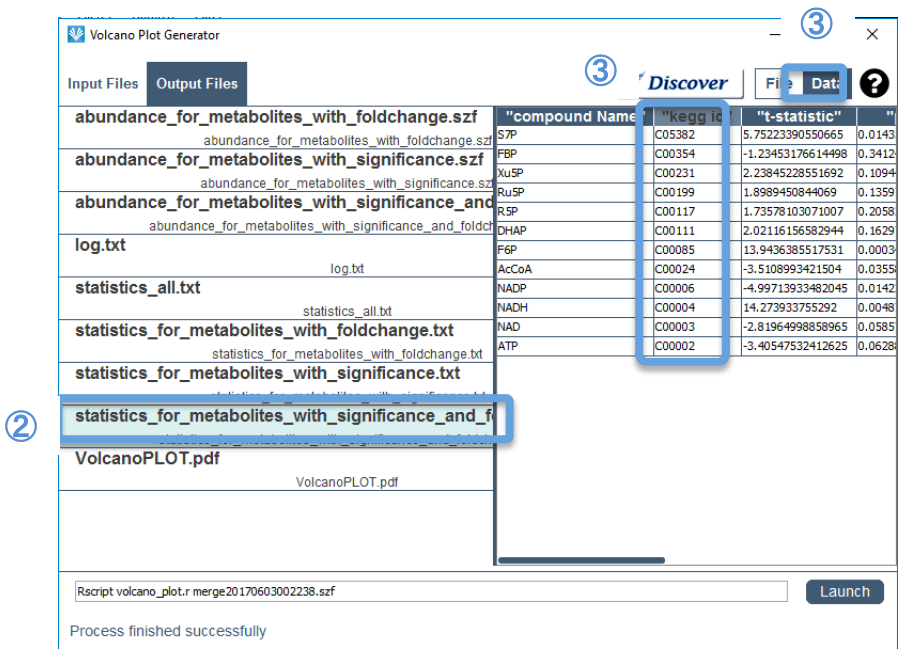
STEP 5. Select significant metabolite list from Volcano Plot Generator analysis results and send the list to other gadget

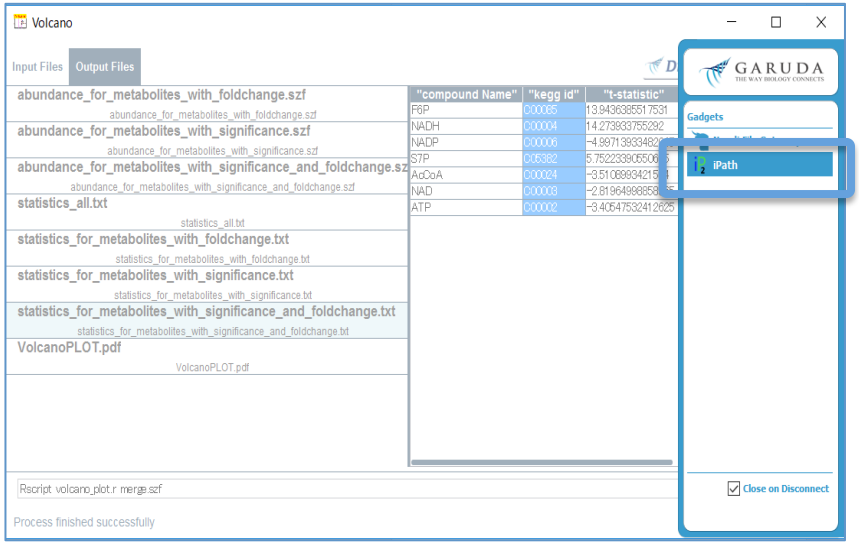
1. Back to results from "**Volcano Plot Generator**" in STEP 2. analysis.

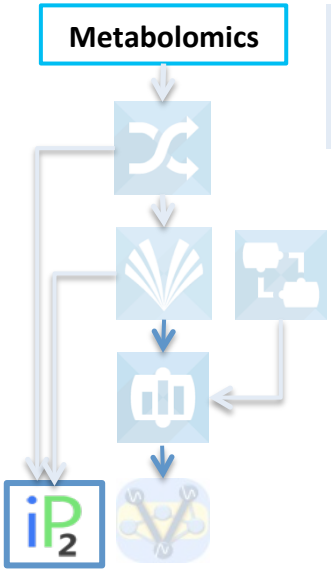
2. Select **File** for statistics for significant metabolites (e.g., statistics_for_metabolites_with_significance_and_foldchange.txt).

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.





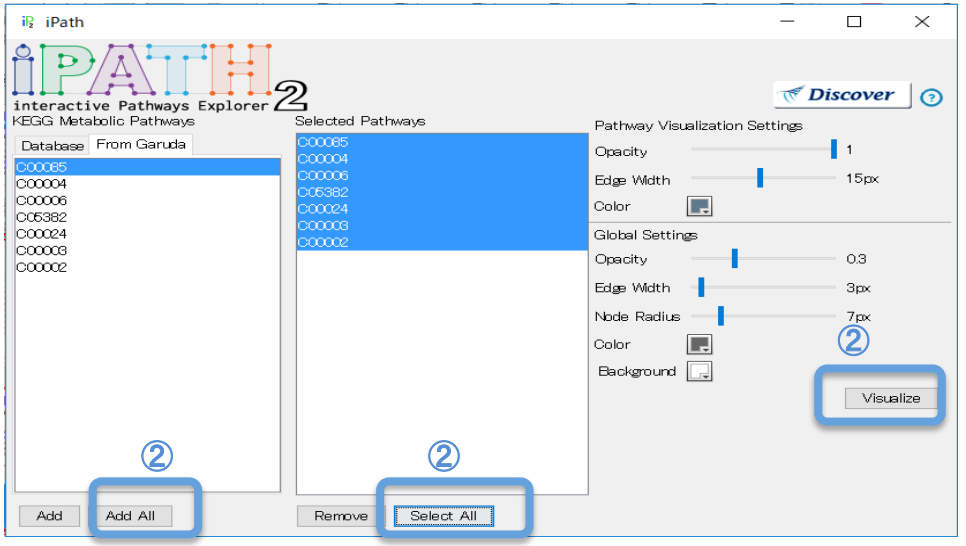


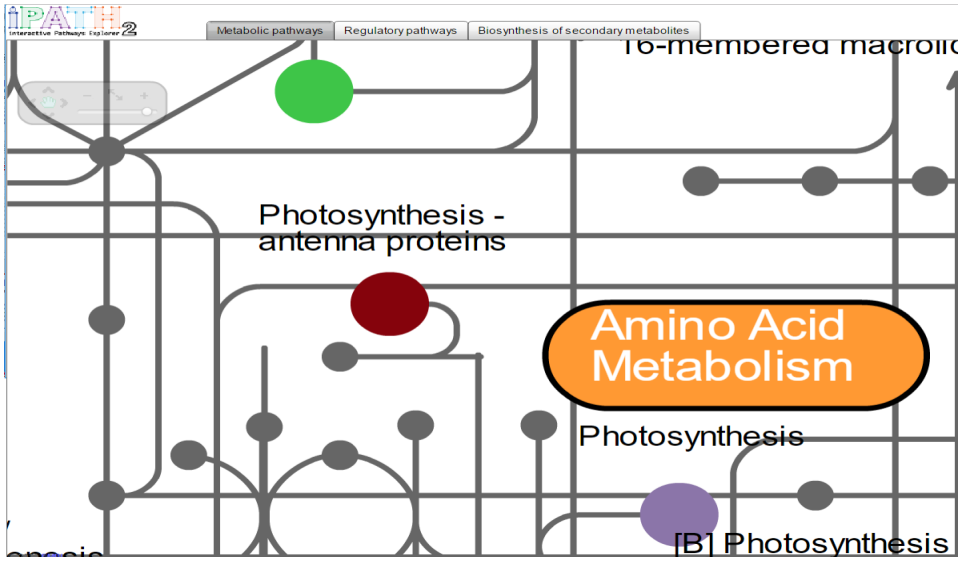
Step 6. Mapping significant compounds on KEGG pathway map

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.

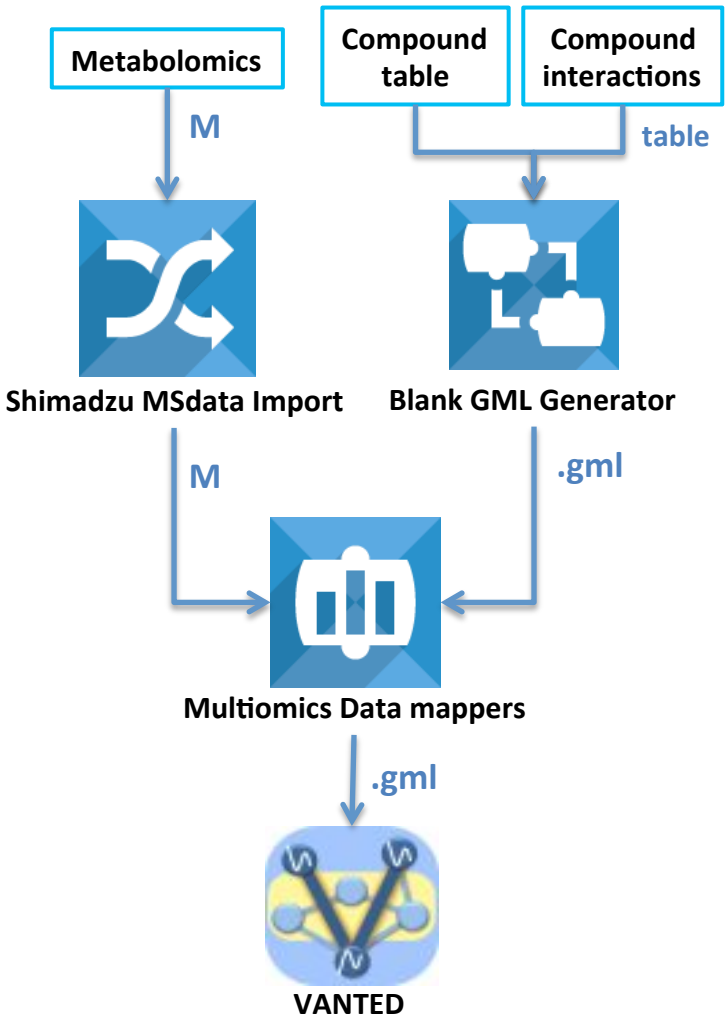
3. Then, please click "**visualize**" button to map and **visualize compounds** on the **KEGG pathway map**.

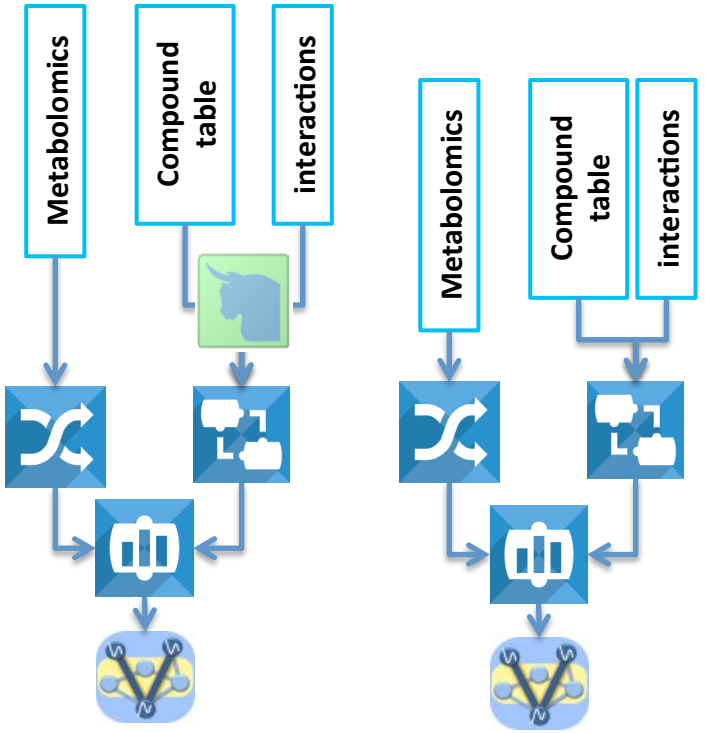




Recipe #2 : Visualize Metabolite Data to Metabolomic Pathway on VANTED

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.





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**

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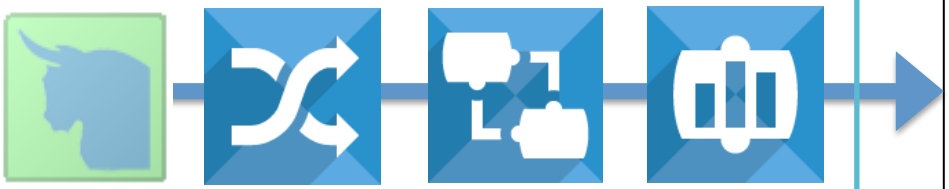
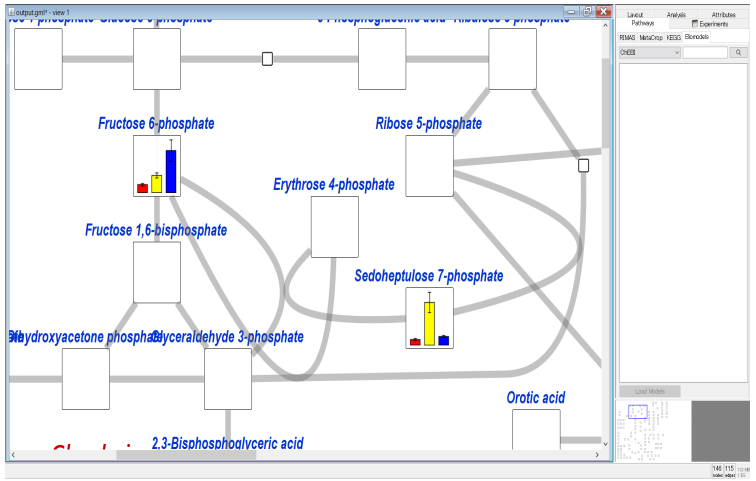
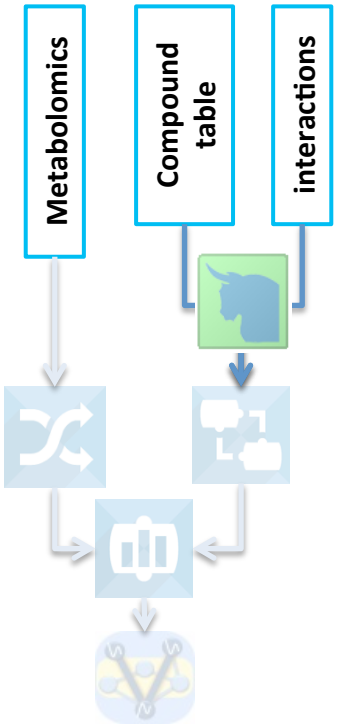


OUTPUT



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



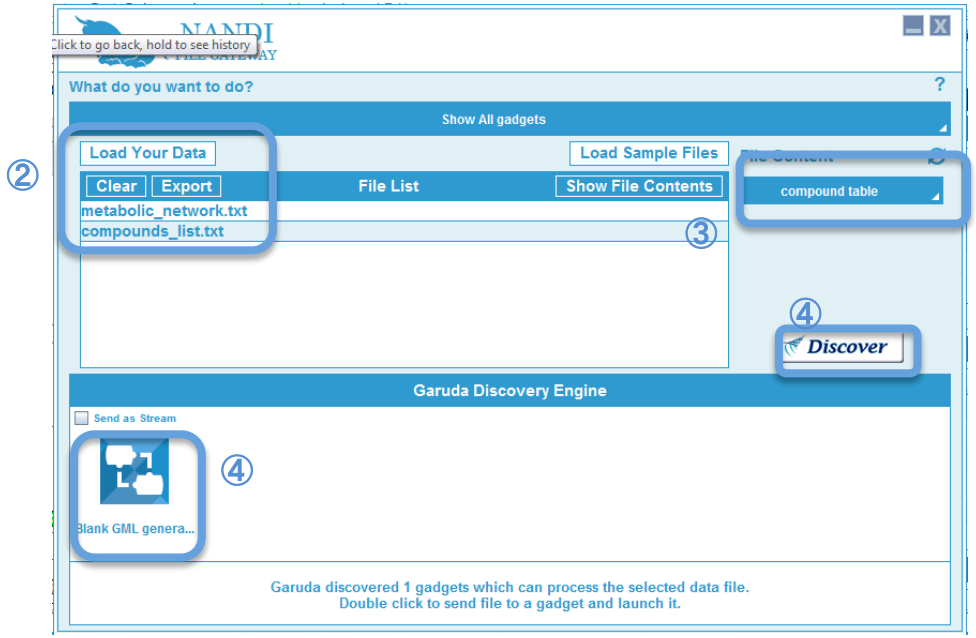
STEP 1. Start with Nandi.

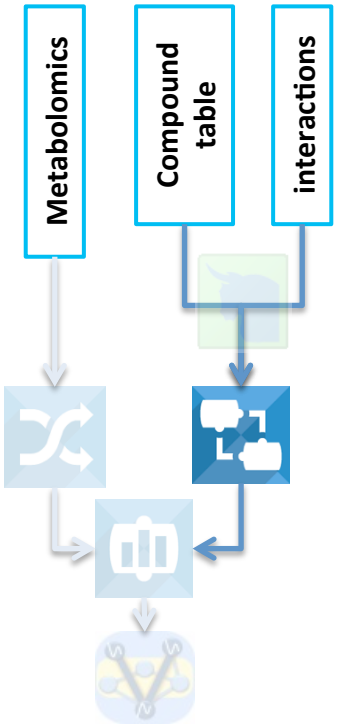
1. Launch the gadget **Nandi** from the Garuda Dashboard (available under StartKit category).

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”**



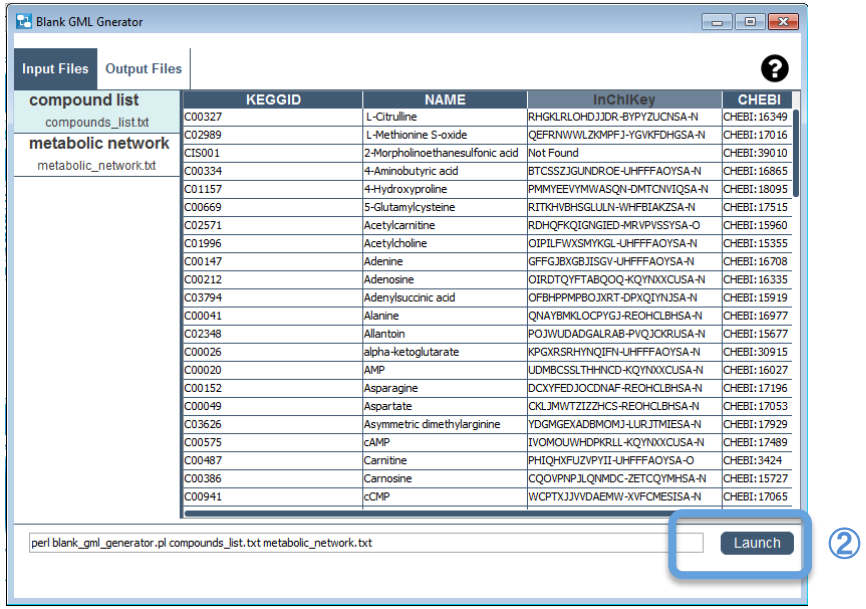


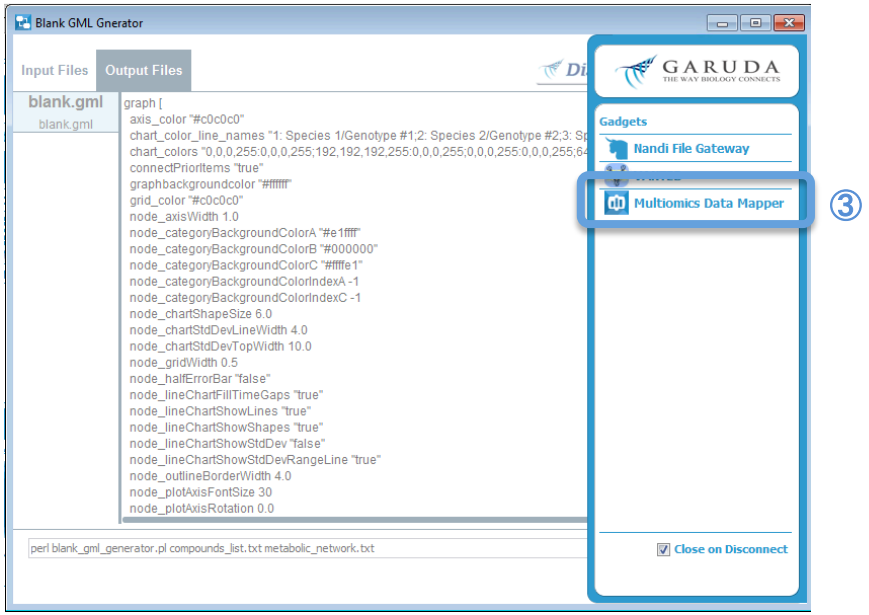
STEP 2. Generate a blank .gml file

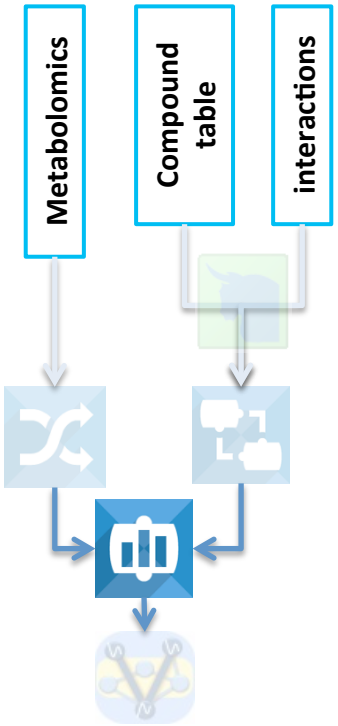
1. From the **Nandi** discovery panel, select and double-click the **"Blank GML Generator"** gadget. Garuda will launch the gadget and send the data files to the gadget

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".







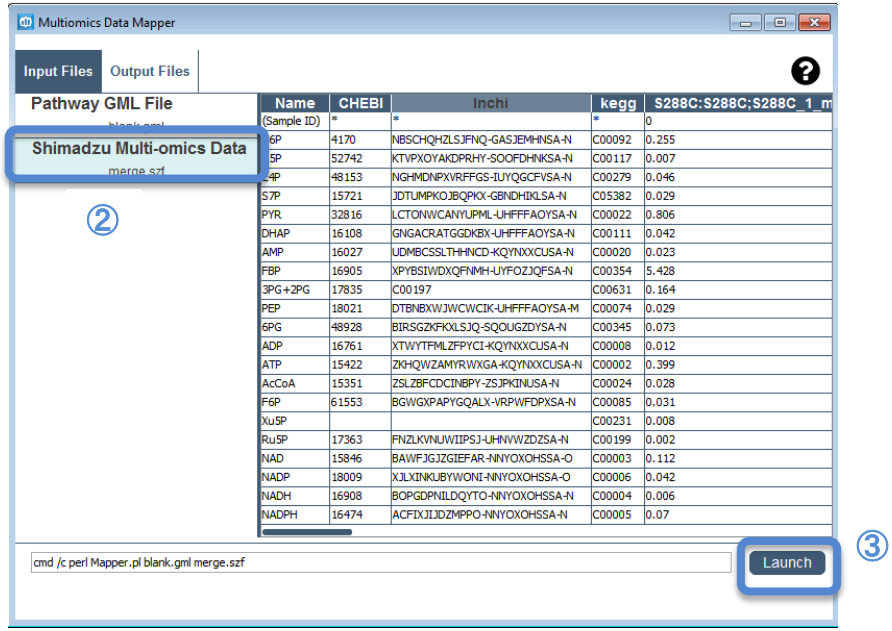
STEP 3. Merge the blank .gml file generated in STEP 2 with metabolome abundance data.

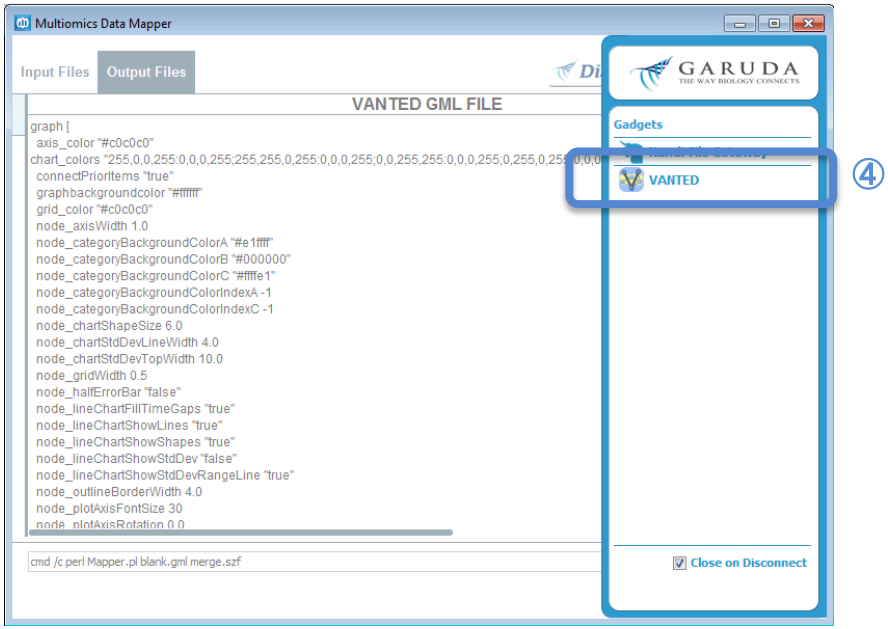
1. On clicking **Discover** in the last action in STEP 2, a list of gadgets which can process the blank .gml file generated in STEP 2 are displayed. Select and double-click the **"Multiomics Data Mapper"** gadget. Garuda will launch the gadget and send the blank .gml file to the gadget

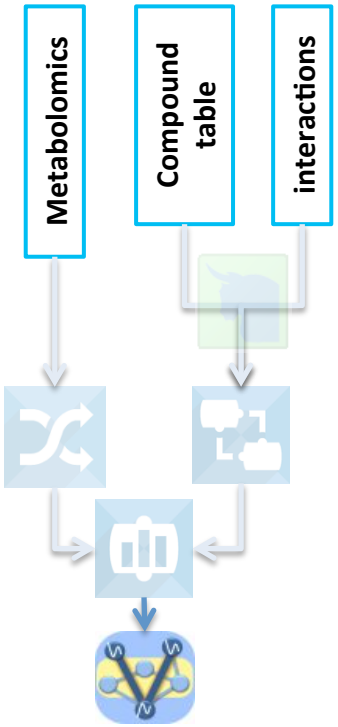
2. In the same manner to **RECIPES #1**, please use "**Shimadzu MSdata Import**" to format metabolome abundance data and upload the formatted abundance data ton "**Multiomics Data Mapper**" gadget.

3. Click "**Launch**" to merge metabolome abundance with the blank .gml file generated from STEP 2.

4. Select **File** and click **Discover**. You can find **VANTED** gadget.



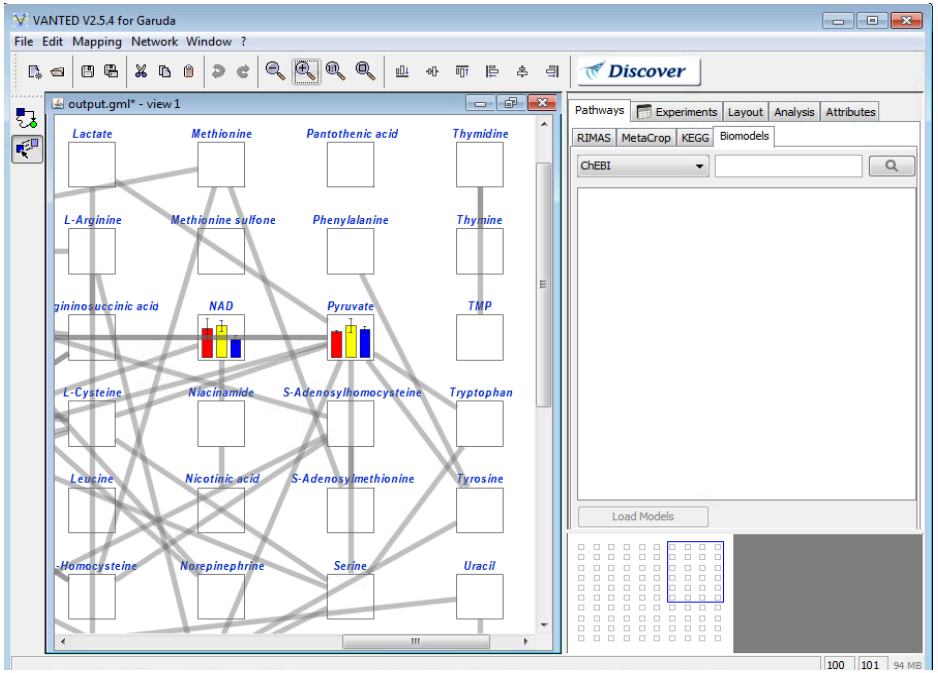




STEP 4. Visualize metabolome abundance on blank metabolome network through VANTED.

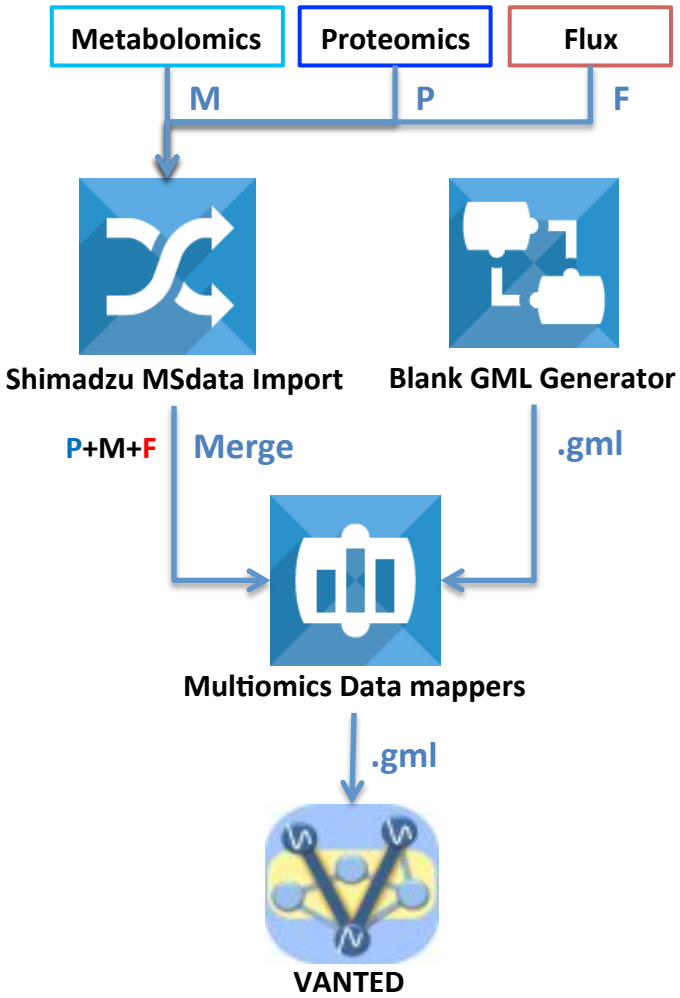
On clicking **Discover** in the last action in STEP3, a list of gadgets which can process merged .gml file are displayed.

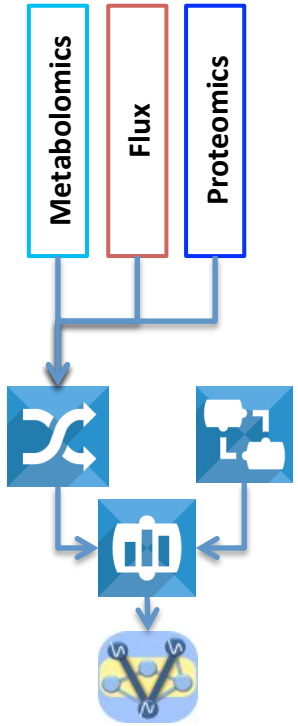
1. Select **VANTED** gadget and double click to launch VANTED gadget.
   Garuda will send the merged .gml file to VANTED and open it for **visualization.**



Recipe #3 : Visualize Multiomics Data to VANTED pathway

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





Recipe #3 : Visualize Multiomics Data to VANTED pathway

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

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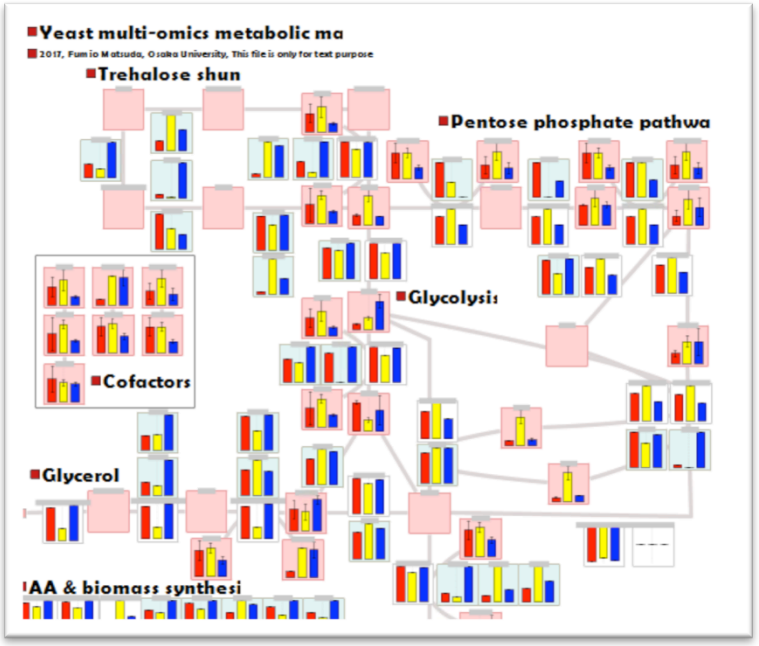
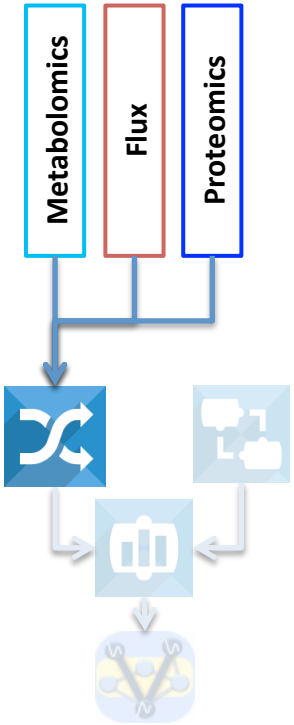
OUTPUT



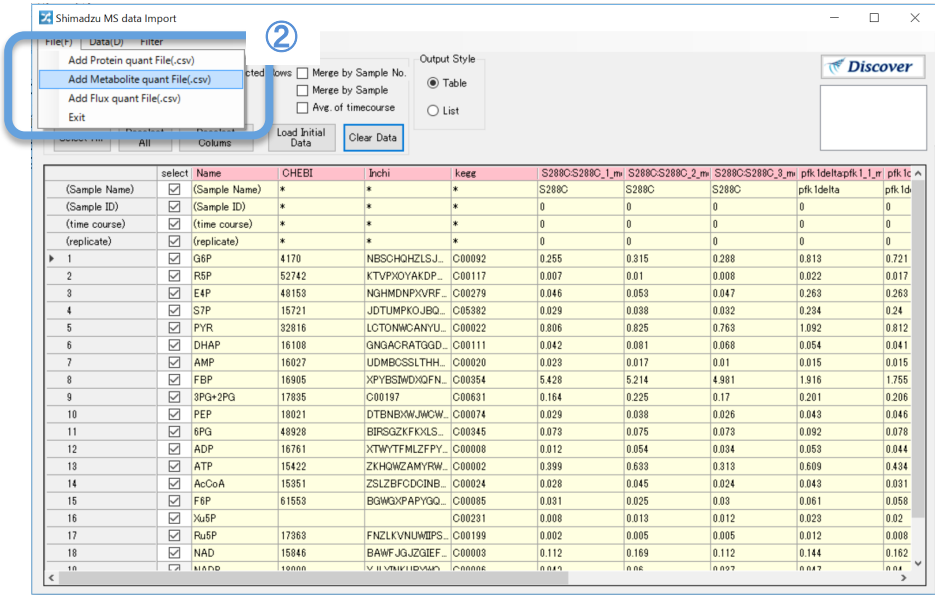


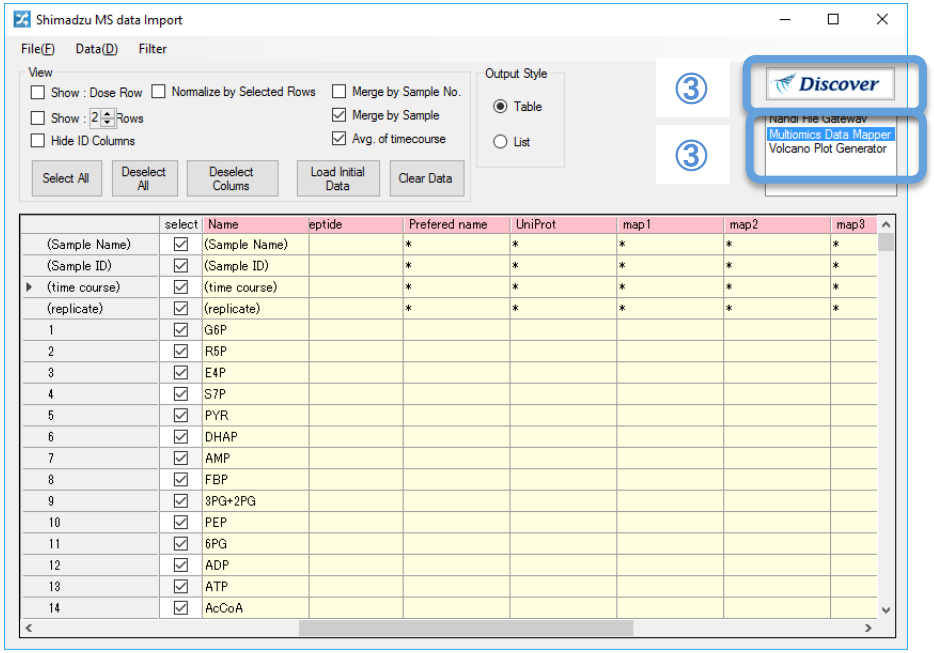
STEP 1. Format Shimadzu multiomics datasets for downstream analysis gadgets

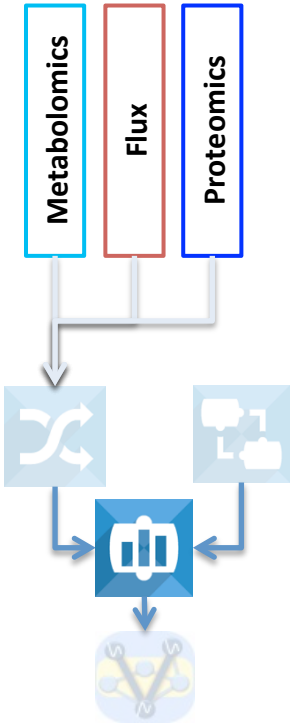
1. From the Garuda dashboard, select and double-click the **"Shimadzu MSdata Import"** gadget to launch the gadget.

2. Click "**File**" and one of the following menu:
   "**Add Metabolite Quant File**"
   "**Add Flux Quant File**",
   "**Add Protein Quant File**"
   to select and import (merge) the sample metabolome abundance data, flux data, and proteome abundance data, respectively (**Sample files:**
   "Sample_multi_omics_metabolome_data.csv",
   "Sample_multi_omics_metabolic_flux.csv", and
   "Sample_multi_omics_proteome_data.csv",
   respectively, in
   ShimadzuGadgets_SampleData> ShimadzuMSdataImport).

3. Click "**Discover**" to list up gadget for downstream analysis. Select and double click **Gadget (**in this recipe, **"Multiomics Data Mapper")**. You can upload the formatted data on the selected gadget.







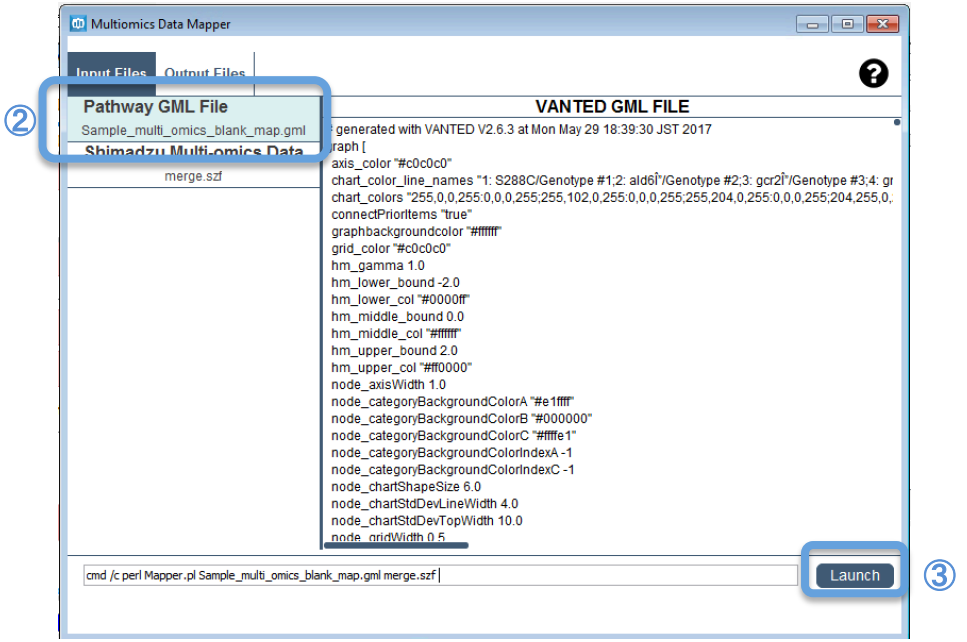
STEP 2: Merge multi-omics data on blank molecular network

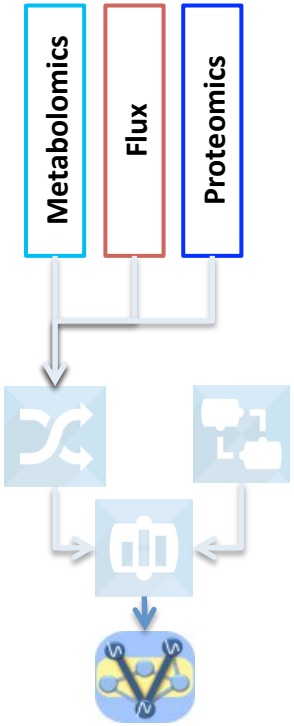
1. From "**Shiamdzu MSdata Import**", select and double-click the "**Multiomics Data Mapper**" gadget. Garuda will launch the gadget and send the data files to the gadget

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.**