

Volcano Plot (Input)



This gadget generates volcano plot visualization and calculates statistics of volcano plot analysis from metabolome abundance (lcms) data of Shimadzu.

Volcano Plot Generator

Input Files | Output Files

(1) Shimadzu Omics Data
test_metabolome_a.szf

(2) Configuration

Double click a rows to load files

compound name	ChEBI	Inchi	KEGG_COMPOUND	S2
(Sample No)	*	*	*	0
G6P	CHEBI:4170	NBSCHQHZLSJFNQ-GASJEMHNSA-N	C00092	0.255
R5P	CHEBI:52742	KTVPXOYAKDPRHY-SOOFDHNKSA-N	C00117	0.007
E4P	CHEBI:48153	NGHMDNPXVRFPGS-IUYQGCVFSA-N	C00279	0.046
S7P	CHEBI:15721	JDTUMPKOJBQPKX-GBNDHIKLSA-N	C05382	0.029
PYR	CHEBI:32816	LCTONWCANYUPML-UHFFFAOYSA-N	C00022	0.806
DHAP	CHEBI:16108	GNGACRATGGDKBX-UHFFFAOYSA-N	C00111	0.042
AMP	CHEBI:16003	UNAPROBETUNIBP-KOYANXUSA-N	C00020	0.023
FBP			C00354	5.428
3PG+2PG			C00631	0.164
PEP	CHEBI:18021	DTBNBXWJWCWCIK-UHFFFAOYSA-M	C00074	0.025
6PG	CHEBI:48928	BIRSGZKFKXLSJQ-SQOUGZDYSA-N	C00345	0.073
ADP	CHEBI:16761	XTWYTFMLZFPYCI-KQYNXXCUSA-N	C00008	0.012
ATP	CHEBI:15422	ZKHQWZAMYRWXGA-KQYNXXCUSA-N	C00002	0.395
AcCoA	CHEBI:15351	ZSLZBFCDCINBPY-ZSJKINUSA-N	C00024	0.028
F6P	CHEBI:61553	BGWGXPAYPYGALX-VRPWFDPXSA-N	C00085	0.031
Xu5P			C00231	0.008
Ru5P	CHEBI:17363	FNZLKVNUWIIPSJ-UHNVWZDZSA-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

The gadget require one input file; **Shimazu metabolome abundance data** (e.g., test_metabolome_a.szf)

Sample File:

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

Required R and R 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.

Volcano Plot (Input)

(parameter settings)

2. Select “control” and “target” samples for Volcano plot 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.

The screenshot shows the 'Volcano Plot Generator' application window. It has two tabs: 'Input Files' and 'Output Files'. Under 'Input Files', there is a section for 'Shimadzu Omics Data' with the file 'test_metabolome_a.szf'. Below this is the 'Configuration' section, which is highlighted with a blue arrow and the instruction '1. Click “Configuration” to open GUI to set the parameters'. The configuration section contains a table for selecting samples as Control or Target, and two input fields for 'p-value' (set to 0.05) and 'Fold Change' (set to 2), both marked as mandatory fields. A blue box highlights the sample selection table, and another blue box highlights the p-value and Fold Change fields. At the bottom, there is a terminal-like window showing the command 'Rscript volcano_plot.r test_metabolome_a.szf' and a 'Launch' button, which is also highlighted with a blue arrow and the instruction '4. Click the bottom to do volcano plot analysis after data upload after data upload and parameter setting'. The status bar at the bottom left indicates 'Connected to Garuda'.

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

```
Rscript volcano_plot.r test_metabolome_a.szf
```

Launch

Connected to Garuda

3. Set threshold value of p-value and that of foldchange for volcano plot 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 analysis after data upload after data upload and parameter setting

Volcano Plot (Output)

The screenshot shows the 'Volcano Plot Generator' application window. The title bar includes the application name and standard window controls. Below the title bar, there are tabs for 'Input Files' and 'Output Files', with 'Output Files' currently selected. To the right of the tabs are buttons for 'Discover', 'File', 'Data', and a help icon. The main content area is divided into two sections. The top section, labeled 'log.txt', contains an error message: 'Error:A column for compound ID is selected as Control sample. Please do not select ID colu' and 'Process terminated.'. The bottom section is a large empty area labeled 'Results Panel'. At the bottom of the window, there is a command line input field containing 'Rscript volcano_plot.r test_metabolome_a.szf' and a 'Launch' button. Below the command line, a status message reads 'Process finished successfully'.

Log file to check if the analysis runs successfully

After “Launch” the analysis, the log.txt file would be generated to see if the analysis results are successfully generated

- “log.txt” is the log file of the analysis run results. If you see any error message, please revisit if your input file setting is correct.

Volcano Plot (output)

The screenshot shows the 'Volcano Plot Generator' application window. It has two tabs: 'Input Files' and 'Output Files'. The 'Output Files' tab is active, showing a list of files generated from the analysis. A blue box highlights 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'. An arrow points to the first file with the text 'Double click a row to download files'. To the right, a 'Results Panel' displays a table with columns: 'compound Name', 'kegg id', 't-statistic', and a fourth column. The table lists various metabolites like G6P, R5P, E4P, S7P, PYR, DHAP, AMP, FBP, 3PG+2PG, YEP, 3PG, ADP, ATP, AcCoA, 6P, Ru5P, NAD, NADP, NADH, and NADPH. At the bottom, there is a terminal window showing the command 'Rscript volcano_plot.r test_metabolome_a.szf' and a 'Launch' button. A status bar at the bottom indicates 'Process finished successfully'.

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	C00382	-16.1711972751795	0.001
PYR			
DHAP			
AMP			
FBP	C00354	1.4978891945213	0.255
3PG+2PG	C00631	-2.42061092514349	0.121
YEP	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
Ru5P	C00231	-0.253616731056512	0.818
Ru5P	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

Statistics from Volcano plot 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.

Volcano Plot (output)

The screenshot shows the 'Volcano Plot Generator' application window. The 'Output Files' tab is active, displaying a list of generated files. A blue box highlights three files: 'abundance_for_metabolites_with_foldchange.szf', 'abundance_for_metabolites_with_significance.szf', and 'abundance_for_metabolites_with_significance_and_foldchange.szf'. 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' displays a table with columns for 'compound names', 'ChEBI', and 'Inchi'. The table contains several rows of metabolite data, including ATP, ADP, AMP, and NADPH. At the bottom of the window, a text box contains the command 'Rscript volcano_plot.r test_metabolome_a.szf' and a 'Launch' button. A status message at the bottom left reads 'Process finished successfully'.

"compound names"	"ChEBI"	"Inchi"
*	*	*
ATP	CHEBI:48153	NGHMDNPXVRFSG-IUYQGCFV
ADP	CHEBI:16761	XTWYTFMLZFPYCI-KQYNXXCU
AMP	CHEBI:15721	JDTUMPKOJBQPKX-GBNDHIKL
NADP		IYOXOHS
AcCoA		RPWFDF
ATP	CHEBI:15422	ZKHQWZAMYR WXGA-KQYNXX
NADPH	CHEBI:16474	ACFIXJIJDZMPPO-NNYOXOHS

Metabolome abundance data from Volcano plot 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 foldchange greater than user defined threshold value.
- “abundance_for_metabolites_with_significance_and_foldchange.szf” is abundance for metabolites with p-value and foldchange that are lower and greater than user defined threshold values, respectively.

Volcano Plot (output)

This gadget generates volcano plot visualization.

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
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

