

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

Shimadzu Omics Data
test_metabolome_a.szf

Configuration

Double click a rows to load files

File is displayed here

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	NGHMDNPXVRFFGS-IUYQGCFSVA-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:16033	UNPUBBLIBPUB-UNPUBBLIBPUB-N	C00020	0.023
FBP			C00354	5.428
3PG+2PG			C00631	0.164
PEP	CHEBI:18021	DTBNBXWJWCWCIK-UHFFFAOYSA-M	C00074	0.029
6PG	CHEBI:48928	BIRSGZKFKXLSJQ-SQOUGZDYSA-N	C00345	0.073
ADP	CHEBI:16761	XTWYTFMLZFPYCI-KQYNXXCUSA-N	C00008	0.012
ATP	CHEBI:15422	ZKHQWZAMRWXGA-KQYNXXCUSA-N	C00002	0.399
AcCoA	CHEBI:15351	ZSLZBFDCINBPY-ZSJKINUSA-N	C00024	0.028
F6P	CHEBI:61553	BGWGXPAYPYGQALX-VRPWFDPXSA-N	C00085	0.031
Xu5P			C00231	0.008
Ru5P	CHEBI:17363	FNZLKVNWIIPSJ-UHNVWZDZSA-N	C00199	0.002
NAD	CHEBI:15846	BAWFJGJGIEFAR-NNYOXOHSSA-O	C00003	0.112
NADP	CHEBI:18009	XJLXINKUBYWONI-NNYOXOHSSA-O	C00006	0.042
NADH	CHEBI:16908	BOPGDPNILDQYTO-NNYOXOHSSA-N	C00004	0.006

Rscript volcano_plot.r test_metabolome_a.szf

Launch

Connected to Garuda

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 **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 a top bar with a logo and window controls. Below is a tabbed interface with 'Input Files' and 'Output Files'. The 'Input Files' tab is active, showing 'Shimadzu Omics Data' and a file named 'test_metabolome_a.szf'. A 'Configuration' section is highlighted with a blue arrow and annotation 1. The 'Configuration' section contains a table for selecting samples and two input fields for p-value and Fold Change, both with blue arrows and annotation 3. The table has columns for 'Sample', 'Control*', and 'Target*'. The 'p-value' field is set to 0.05 and the 'Fold Change' field is set to 2. A red asterisk indicates these are mandatory fields. At the bottom, there is a command line field containing 'Rscript volcano_plot.r test_metabolome_a.szf' and a 'Launch' button, both with blue arrows and annotation 4.

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 *

Fold Change *

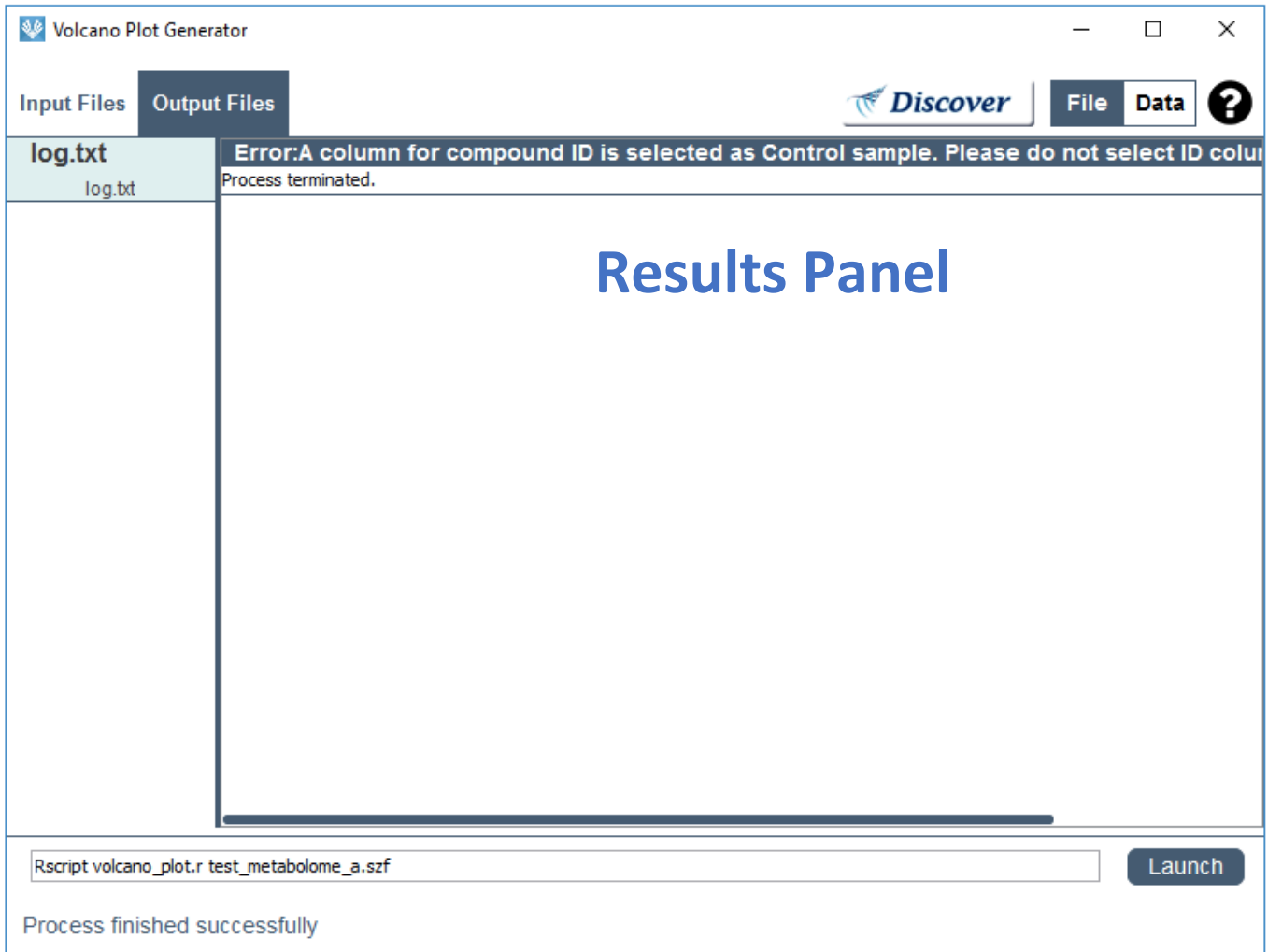
* Mandatory Fields

Rscript volcano_plot.r test_metabolome_a.szf

Launch

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)



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)

Volcano Plot Generator

Input Files

Output Files

Discover

File

Data

?

abundance_for_metabolites_with_foldchange.szf	"compound Name"	"kegg id"	"t-statistic"	
abundance_for_metabolites_with_foldchange.szf	G6P	C00092	-13.3306576525995	0.003
abundance_for_metabolites_with_significance.szf	R5P	C00117	-0.817068173972164	0.486
abundance_for_metabolites_with_significance.szf	E4P	C00279	-12.9043732505126	0.000
abundance_for_metabolites_with_significance_and_foldchange.szf	S7P	C005382	-16.171197751795	0.000
log.txt	PYR			
log.txt	DHAP			
statistics_all.txt	AMP			
statistics_all.txt	FBP	C00354	1.4978891945213	0.255
statistics_for_metabolites_with_foldchange.txt	3PG+2PG	C00631	-2.42061092514349	0.121
statistics_for_metabolites_with_foldchange.txt	PEP	C00074	-2.56191032522519	0.113
statistics_for_metabolites_with_significance.txt	3PG	C00345	-1.85185763881223	0.172
statistics_for_metabolites_with_significance.txt	ADP	C00008	-11.0953007490424	0.000
statistics_for_metabolites_with_significance_and_foldchange.txt	ATP	C00002	-5.64721273310225	0.019
VolcanoPLOT.pdf	AcCoA	C00024	-6.21822952748817	0.003
VolcanoPLOT.pdf	6P	C00085	7.53279330473999	0.003
	Ku5P	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

Results Panel

Double click a row to download files

Rscript volcano_plot.r test_metabolome_a.szf

Launch

Process finished successfully

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' web application. The 'Output Files' tab is active, displaying a list of generated files. A blue box highlights the first three files: 'abundance_for_metabolites_with_foldchange.szf', 'abundance_for_metabolites_with_significance.szf', and 'abundance_for_metabolites_with_significance_and_foldchange.szf'. An arrow points to the first file with the text 'Double click a row to download files'. To the right, the 'Results Panel' displays a table of metabolite data.

"compound names"	"ChEBI"	"Inchi"
*	*	*
ATP	CHEBI:48153	NGHMDNPXVRFSG-IUYQGCFV
ADP	CHEBI:16761	XTWYTFMLZFPYCI-KQYNXXCU
G6P	CHEBI:15721	JDTUMPKOJBQPKX-GBNDHIKL
NADP		IYOXOHS
G6P		RPWFDF
AcCoA		ASJEMHN
ATP	CHEBI:15422	ZKHQWZAMYR-WXGA-KQYNXX
NADPH	CHEBI:16474	ACFIXIJDZMPPPO-NNYOXOHS

At the bottom of the interface, 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'.

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	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

