

Shimadzu MSdata Import

2017 July



What's New !

2017.07 v1.0.1 release

- [File] Add loadable text file format
 - LabSolutions : .txt file
 - LabSolutions Insight : .csv file

Release Note:

2017.06 v1.0 release

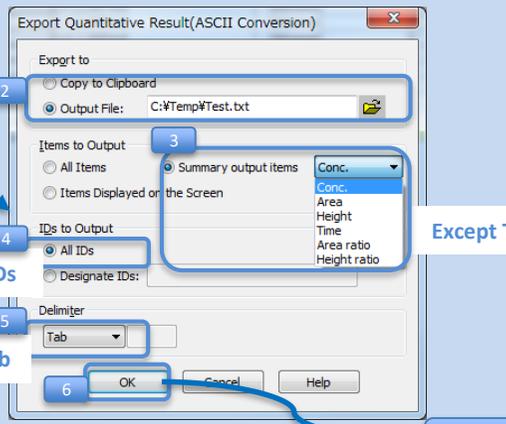
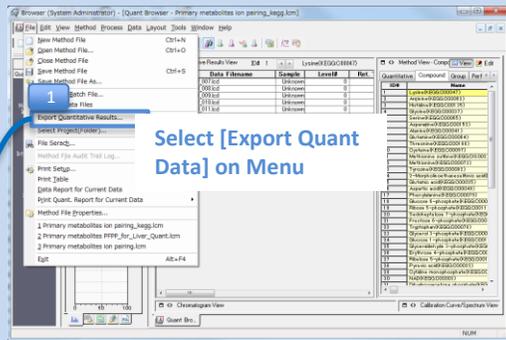


PREPARE INPUT DATA

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

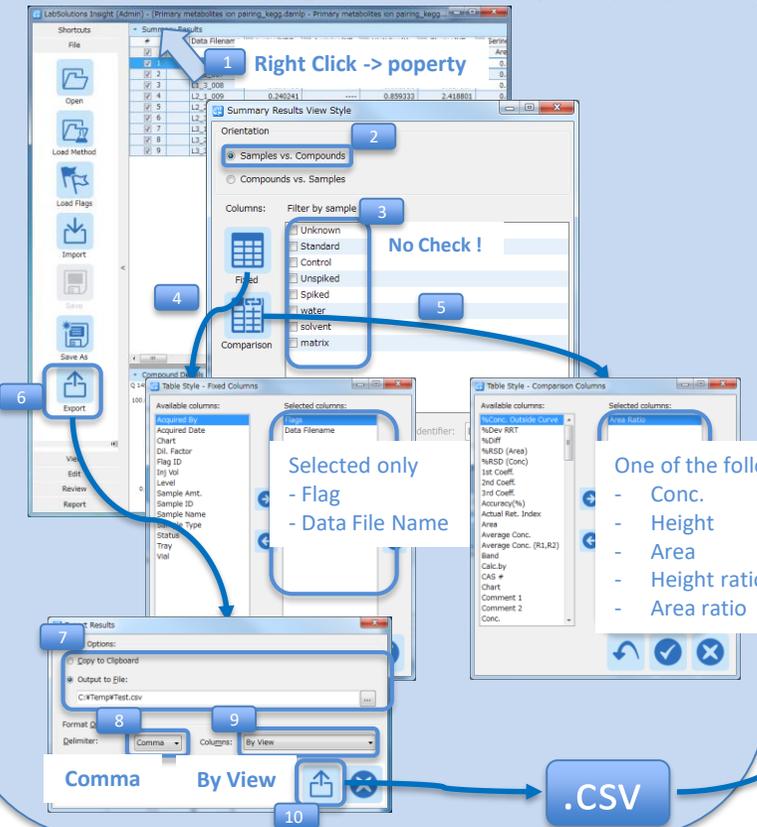
Shimadzu MS data (.lcb or .lcm and .lcd)

LabSolutions - Quant browser



.txt

LabSolutions Insight - Summary display





“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)

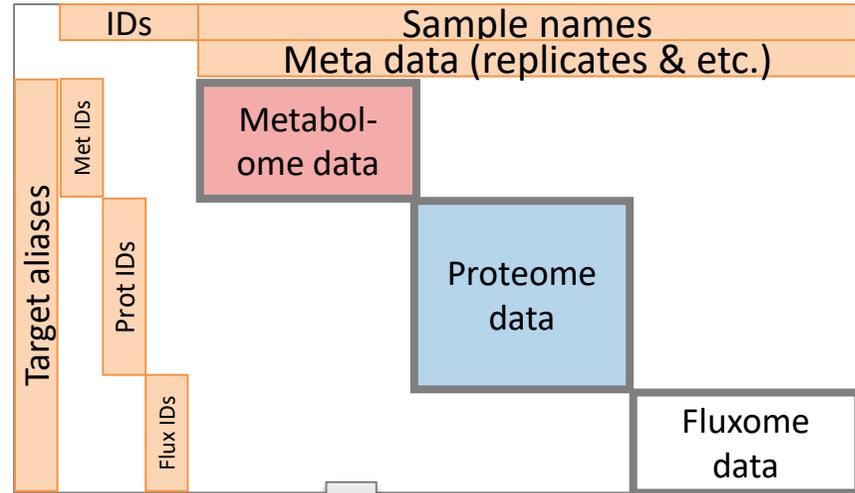


- Merge dataset
- Normalize data
- Average timecourse data
- Imputate data
- Select compounds

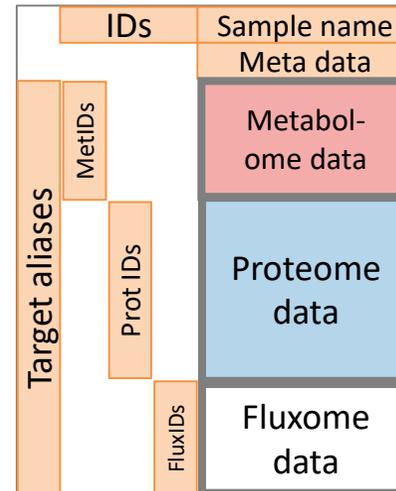
OUTPUT

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

(.szf)



Merge dataset





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 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
▶ (Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	S288C
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	0
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	0
(dose)	<input checked="" type="checkbox"/>	(dose)	*	*	*	0
1	<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLSJ...	C00092	0.255
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPXOYAKDP...	C00117	0.007

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	S288C	pkf.Idelta	pkf.Idelta	pkf
▶ (Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	S288C	S288C	S288C	pkf.Idelta	pkf.Idelta	pkf
(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	0.721	0.5	
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPXOYAKDP...	C00117	0.007	0.01	0.008	0.017	0.6	

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	avg.S288C
▶ (Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	S288C
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	0
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	0
1	<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLSJ...	C00092	0.4507777777777777
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPXOYAKDP...	C00117	0.0157777777777777
3	<input checked="" type="checkbox"/>	EXP	40153	NGSHKAPVORF...	C00279	0.1021111111111111
4	<input checked="" type="checkbox"/>	SIP	19721	LCTUMKFOJSD...	C00192	0.1802222222222222
5	<input checked="" type="checkbox"/>	PYR	32816	LCTONMAGNYL...	C00022	0.5807777777777777
6	<input checked="" type="checkbox"/>	DHAP	16108	ONGACRATOGG...	C00111	0.0711111111111111
7	<input checked="" type="checkbox"/>	AMP	16027	UDMBCSSLTH...	C00020	0.0145555555555555
8	<input checked="" type="checkbox"/>	FBP	16905	JPFYBSMDGDF...	C00344	0.3740000000000000
9	<input checked="" type="checkbox"/>	SPG+SPG	17835	C00187	C00024	0.1802222222222222
10	<input checked="" type="checkbox"/>	PEP	18021	DTBNSJNWKW...	C00074	0.0594444444444444
11	<input checked="" type="checkbox"/>	SPO	48928	BIRGZFKXLS...	C00045	0.0155555555555555
12	<input checked="" type="checkbox"/>	ADP	16761	JQWYTMZLZFY...	C00080	0.015
13	<input checked="" type="checkbox"/>	ATP	16022	ZLHGZANRHW...	C00022	0.0241111111111111
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZDFCCJNB...	C00024	0.0200000000000000
15	<input checked="" type="checkbox"/>	FBP	61553	BGWSKAPFYQ...	C00005	0.0877777777777777
16	<input checked="" type="checkbox"/>	%ASP	17883	FNZLIVNMGPS...	C00199	0.0077777777777777
17	<input checked="" type="checkbox"/>	NAD	15846	BNWFJLJDFE...	C00003	0.1011111111111111
18	<input checked="" type="checkbox"/>	NADP	18009	XJLQKLUYQW...	C00006	0.0175555555555555



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.

Loadable columns < about 650 columns

Sample File:

Sample file to test is available under **Samples > Shimadzu MSdata Import**

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

The screenshot shows the 'Shimadzu MS data Import' window. A blue box highlights the 'Add Metabolite quant File(.csv)' option in the 'Data(D)' menu. Below the menu, there are checkboxes for 'Merge by Sample No.', 'Merge by Sample', and 'Avg. of timecourse', and radio buttons for 'Table' (selected) and 'List'. A 'Discover' button is also visible. The main area displays a data table with columns for 'select', 'Name', 'CHEBI', 'Inchi', 'kegg', and three 'S288C' columns, followed by 'pkf Idelta' and 'pkf Id'. A white box with blue text points to the table, stating 'A imported data table is displayed here'.

	select	Name	CHEBI	Inchi	kegg	S288C:S288C_1_mv	S288C:S288C_2_mv	S288C:S288C_3_mv	pkf Idelta	pkf Id
(Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	S288C	S288C	S288C	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	0.721
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPXQYAKDP...	C00117	0.007	0.01	0.008	0.022	0.017
3	<input checked="" type="checkbox"/>	E4P	48153	NGHMDNPKXVRF...	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	16097	UIMRPOSSITW...	C00090	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	ZSLZBFCDCINB...	C00024	0.028	0.045	0.024	0.043	0.031
15	<input checked="" type="checkbox"/>	F6P	61553	BGWGXPPAPYG...	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	15808	YUYNKUPYWD...	C00005	0.043	0.06	0.037	0.047	0.04



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.

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

	select	Name	CHEBI	Inchi	kegg	S289C-S289C_1_m	S289C-S289C_2_m	S289C-S289C_3_m	pkf.Idelta	pkf.1_r	pkf.1c
(Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	S289C	S289C	S289C	pkf.Idelta	pkf.1c	
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0	0	0	0	0	0
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	n	n	n	0	0	0
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*				0	0	0
1	<input checked="" type="checkbox"/>	G6P	4170					8	0.813	0.721	
2	<input checked="" type="checkbox"/>	R5P	52742					8	0.022	0.017	
3	<input checked="" type="checkbox"/>	E4P	48153					7	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	UDMBCSSLTHH...	C00020	0.023	0.017	0.01	0.015	0.015	
8	<input checked="" type="checkbox"/>	FBP	16905	XPYBSIMDXQFN...	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	DTBNBXWJMCW...	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	ZSLZBFCDCINB...	C00024	0.028	0.045	0.024	0.043	0.031	
15	<input checked="" type="checkbox"/>	F6P	61553	BGWGXPAPYQG...	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	BAWFJGJGIEF...	C00003	0.112	0.169	0.112	0.144	0.162	

The screenshot shows the Shimadzu MS data Import window with the data table cleared. The interface includes the same menu options and buttons as the previous screenshot, but the table area is empty.



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 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	p
<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	0	0	0	0	0
<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0	0	0	0	0
<input checked="" type="checkbox"/>	(time course)	*	*	*	0	0	0	0	0
<input checked="" type="checkbox"/>	(replicate)	*	*	*	0	0	0	0	0
<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLSJ...	C00092	0.255	0.315	0.288	0.813	0
<input checked="" type="checkbox"/>	R5P	52742	KTVPXOYAKDP...	C00117	0.007	0.01	0.008	0.022	0
<input checked="" type="checkbox"/>	E4P	48153	NGHMDNPXVRF...	C00279	0.046	0.053	0.047	0.263	0
<input checked="" type="checkbox"/>	S7P	15721	JDTUMPKOJBQ...	C05382	0.029	0.038	0.032	0.234	0
<input checked="" type="checkbox"/>	PYR	32816	LCTONWCANYU...	C00022	0.806	0.825	0.763	1.092	0
<input checked="" type="checkbox"/>	DHAP	16108	GNGACRATGGD...	C00111	0.042	0.081	0.068	0.054	0
<input checked="" type="checkbox"/>	AMP	16027	UOMBCSSLTHH...	C00020	0.023	0.017	0.01	0.015	0
<input checked="" type="checkbox"/>	FBP	16905	XPYBSMWDXQFN...	C00354	5.428	5.214	4.981	1.916	1
<input checked="" type="checkbox"/>	3PG+2PG	17835	C00197	C00631	0.164	0.225	0.17	0.201	0
<input checked="" type="checkbox"/>	PEP	18021	DTENBXWJWCW...	C00074	0.029	0.038	0.026	0.043	0
<input checked="" type="checkbox"/>	6PG	48928	BIRSGZKFKKLS...	C00345	0.073	0.075	0.073	0.092	0
<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY...	C00008	0.012	0.054	0.034	0.053	0
<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW...	C00002	0.399	0.633	0.313	0.609	0
<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFDCINB...	C00024	0.028	0.045	0.024	0.043	0
<input checked="" type="checkbox"/>	F6P	61553	BGWGXPAFYGG...	C00085	0.031	0.025	0.03	0.061	0
<input checked="" type="checkbox"/>	Xu5P		C00231	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	p
<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	0	0	0	0	0
<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0	0	0	0	0
<input checked="" type="checkbox"/>	(time course)	*	*	*	1	1	1	2	0
<input checked="" type="checkbox"/>	(replicate)	*	*	*	0	0	0	0	0
<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLSJ...	C00092	0.255	0.315	0.288	0.813	0
<input checked="" type="checkbox"/>	R5P	52742	KTVPXOYAKDP...	C00117	0.007	0.01	0.008	0.022	0
<input checked="" type="checkbox"/>	E4P	48153	NGHMDNPXVRF...	C00279	0.046	0.053	0.047	0.263	0
<input checked="" type="checkbox"/>	S7P	15721	JDTUMPKOJBQ...	C05382	0.029	0.038	0.032	0.234	0
<input checked="" type="checkbox"/>	PYR	32816	LCTONWCANYU...	C00022	0.806	0.825	0.763	1.092	0
<input checked="" type="checkbox"/>	DHAP	16108	GNGACRATGGD...	C00111	0.042	0.081	0.068	0.054	0
<input checked="" type="checkbox"/>	AMP	16027	UOMBCSSLTHH...	C00020	0.023	0.017	0.01	0.015	0
<input checked="" type="checkbox"/>	FBP	16905	XPYBSMWDXQFN...	C00354	5.428	5.214	4.981	1.916	1
<input checked="" type="checkbox"/>	3PG+2PG	17835	C00197	C00631	0.164	0.225	0.17	0.201	0
<input checked="" type="checkbox"/>	PEP	18021	DTENBXWJWCW...	C00074	0.029	0.038	0.026	0.043	0
<input checked="" type="checkbox"/>	6PG	48928	BIRSGZKFKKLS...	C00345	0.073	0.075	0.073	0.092	0
<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY...	C00008	0.012	0.054	0.034	0.053	0
<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW...	C00002	0.399	0.633	0.313	0.609	0
<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFDCINB...	C00024	0.028	0.045	0.024	0.043	0
<input checked="" type="checkbox"/>	F6P	61553	BGWGXPAFYGG...	C00085	0.031	0.025	0.03	0.061	0
<input checked="" type="checkbox"/>	Xu5P		C00231	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

The screenshot shows the 'Shimadzu MS data Import' window with the 'Impute Missing-data' option highlighted in the 'Data(D)' menu. A secondary dialog box titled 'Missing-data imputa...' is open, showing 'All data' selected under 'target data' and 'Static val' with a value of '0' selected under 'Imputation Val'.

Row	Gene	delta:PFK1-1	pfk1delta:PFK1-1	S288C:Wild-1_metl	S288C:Wild-1_metl	S2
349				1.2472		
350				0.7975		
351	Pdc6_WAGNANE...			0.7098		
352	Pdc6_WGLKPYLF...			#N/A		
353	Pde1_TEDPELIA...			#N/A		
354	Pfk1_AVLEFTPE...			#N/A		
355	Pfk2_GWSAEGG...	1.2335				
356	Pfk2_NAVSTKPT...	2.1618				

Select **“Impute Missing-data”** to impute missing-data

After the setting, click **“OK”** to impute missing data

The screenshot shows the 'Shimadzu MS data Import' window with 'Table' selected under 'Output Style'. The data table below shows that the previously missing values (NA) have been imputed with the value '0'.

Row	Gene	delta:PFK1-1	pfk1delta:PFK1-1	S288C:Wild-1_metl	S288C:Wild-1_metl	S2
349				1.2472		
350				0.7975		
351	Pdc6_WAGNA...			0.7098		
352	Pdc6_WGLKPYLF...			0		
353	Pde1_TEDPELIA...			0		
354	Pfk1_AVLEFTPE...			0		
355	Pfk2_GWSAEGG...	1.2335				
356	Pfk2_NAVSTKPT...	2.1618				

“NA” are imputed by **“0”** (in this example)



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.

Click check box of “Average of Time course per data” to calculate mean value

select	Name	S288C-S288C_1_m	S288C-S288C_2_m	S288C-S288C_3_m	pkf1delta	pkf1delta	pkf1delta	zvf1delta	zvf1delta	zvf1delta
(Sample Name)	(Sample Name)	S288C	S288C	S288C	pkf1delta	pkf1delta	pkf1delta	zvf1delta	zvf1delta	zvf1delta
(Sample ID)	(Sample ID)									
(time course)	(time course)	1	1	1	2	2	2	3	3	3
(replicate)	(replicate)									
1	G6P	0.255	0.315	0.288	0.813	0.721	0.967	0.247	0.266	0.257
2	R5P	0.007	0.01	0.008	0.022	0.017	0.025	0.03	0.014	0.009
3	E4P	0.046	0.053	0.047	0.263	0.263	0.347	0.049	0.066	0.055
4	S7P	0.029	0.038	0.032	0.234	0.24	0.312	0.051	0.057	0.053
5	PYR	0.806	0.825	0.783	1.092	0.812	1.078	0.815	0.952	0.856
6	DHAP	0.042	0.081	0.068	0.054	0.041	0.075	0.098	0.098	0.083
7	AMP	0.023	0.017	0.01	0.015	0.015	0.012	0.013	0.014	0.012
8	FBP	5.428	5.214	4.981	1.916	1.755	2.431	5.219	4.383	1.747
9	3PG+2PG	0.164	0.225	0.17	0.201	0.206	0.271	0.169	0.184	0.176
10	PEP	0.029	0.038	0.026	0.043	0.046	0.061	0.037	0.039	0.036
11	6PG	0.073	0.075	0.073	0.092	0.078	0.121	0.082	0.069	0.071
12	ADP	0.012	0.054	0.034	0.053	0.044	0.054	0.021	0.023	0.02
13	ATP	0.399	0.633	0.313	0.609	0.434	0.806	0.218	0.22	0.185
14	AcCoA	0.028	0.045	0.024	0.043	0.031	0.045	0.013	0.018	0.013
15	F6P	0.031	0.025	0.03	0.061	0.058	0.071	0.132	0.184	0.144
16	Xu5P	0.008	0.013	0.012	0.023	0.02	0.029	0.034	0.013	0.024
17	Ru5P	0.002	0.005	0.005	0.012	0.008	0.014	0.008	0.005	0.011

select	Name	CHEBI	Inchi	kegg	avg_S288C_S288C	avg_pkf1delta	avg_zvf1delta
(Sample Name)	(Sample Name)	*	*	*			
(Sample ID)	(Sample ID)						
(time course)	(time course)	*	*	*	1	2	3
(replicate)	(replicate)						
1	G6P	4170	NBSCHQHZLSJ...	C00092	0.286	0.839666666666...	0.256666666666...
2	R5P	52742	KTVPXOYAKDP...	C00117	0.009333333333...	0.021333333333...	0.017666666666...
3	E4P	48153	NGHMDNPXVRF...	C00279	0.048666666666...	0.291	0.056666666666...
4	S7P	15721	JDTLMPKOJBO...	C05382	0.033	0.262	0.056666666666...
5	PYR	32816	LCTONWCANYU...	C00022	0.798	0.994	0.874333333333...
6	DHAP	16108	GINGACRATGG...	C00111	0.063666666666...	0.056666666666...	0.093
7	AMP	16027	UDMBCSSLTH...	C00020	0.016666666666...	0.014	0.013
8	FBP	16905	XPYBSMDXQFN...	C00354	5.207666666666...	2.034	3.783
9	3PG+2PG	17835	C00197	C00631	0.186333333333...	0.226	0.176333333333...
10	PEP	18021	DTBNBKWJWCW...	C00074	0.031	0.05	0.037333333333...
11	6PG	48928	BIRSGZKFKXLS...	C00345	0.073666666666...	0.097	0.074
12	ADP	16761	XTWYTFMLZFPY...	C00008	0.039333333333...	0.050333333333...	0.021333333333...
13	ATP	15422	ZKHQWZAMYRW...	C00002	0.448333333333...	0.616333333333...	0.207666666666...
14	AcCoA	15351	ZSLZBFCDCINB...	C00024	0.032333333333...	0.039666666666...	0.014666666666...
15	F6P	61553	BGWGXFAPYGO...	C00005	0.028666666666...	0.063333333333...	0.153333333333...
16	Xu5P			C00231	0.011	0.024	0.029666666666...
17	Ru5P	17363	FNZLKVNUWIPS...	C00199	0.004	0.011333333333...	0.008
18	NAD	15846	BAWF_KJZGIEF...	C00003	0.131	0.144333333333...	0.082



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.

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

(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
S288C		1	0	0.286	0.008333333333	0.048666666666	0.033	0.798	0.063666666666	0.016666666666	5.207666666667	0.186333333333	0.031	0.073666666666	0.033333333333	0.448333333333	0.032333333333	0.028666666666	0.011	0.004
		2	0	0.833666666666	0.021333333333	0.056666666666	0.262	0.994	0.056666666666	0.014	2.034	0.226	0.05	0.097	0.050333333333	0.616333333333	0.039666666666	0.063333333333	0.024	0.008
		3	0	0.256666666666	0.017666666666	0.056666666666	0.053666666666	0.874333333333	0.093	0.013	3.783	0.176333333333	0.037333333333	0.074	0.021333333333	0.207666666666	0.014666666666	0.153333333333	0.023666666666	0.008

Discover

(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
S288C		1	0	0.286	0.008333333333	0.048666666666	0.033	0.798	0.063666666666	0.016666666666	5.207666666667	0.186333333333	0.031	0.073666666666	0.033333333333	0.448333333333	0.032333333333	0.028666666666	0.011	0.004
		2	0	0.833666666666	0.021333333333	0.056666666666	0.262	0.994	0.056666666666	0.014	2.034	0.226	0.05	0.097	0.050333333333	0.616333333333	0.039666666666	0.063333333333	0.024	0.008
		3	0	0.256666666666	0.017666666666	0.056666666666	0.053666666666	0.874333333333	0.093	0.013	3.783	0.176333333333	0.037333333333	0.074	0.021333333333	0.207666666666	0.014666666666	0.153333333333	0.023666666666	0.008



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.

Click "List" at "Output Style" to output list of compound ids

Enter the "kegg" column

	select	Name	CHEBI	Inchi	kegg	Locus id	Peptide	Preferred 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	NBSCHQHZLSJ...	C00092				
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPXOYAKDP...	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	DTBENXWJWCW...	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	BGWGXPAFYGG...	C00085				



Discover

Output Style

Table

List

	select	Name	CHEBI	Inchi	kegg	Locus id	Peptide	Preferred 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	NBSCHQHZLSJ...	C00092				
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPXOYAKDP...	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	DTBENXWJWCW...	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	BGWGXPAFYGG...	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

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

Discover

Nanol File Gateway
Multiomics Data Mapper
Volcano Plot Generator

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

select	Name	peptide	Prefered name	UniProt	map1	map2	map3
<input checked="" type="checkbox"/>	(Sample I						*
<input checked="" type="checkbox"/>	(Sample II						*
<input checked="" type="checkbox"/>	(time cour						*
<input checked="" type="checkbox"/>	(replicate)						*
<input checked="" type="checkbox"/>	G6P						
<input checked="" type="checkbox"/>	R5P						
<input checked="" type="checkbox"/>	E4P						
<input checked="" type="checkbox"/>	S7P						
<input checked="" type="checkbox"/>	PYR						
<input checked="" type="checkbox"/>	DHAP						
<input checked="" type="checkbox"/>	AMP						
<input checked="" type="checkbox"/>	FBP						
<input checked="" type="checkbox"/>	3PG+2PG						
<input checked="" type="checkbox"/>	PEP						
<input checked="" type="checkbox"/>	6PG						
<input checked="" type="checkbox"/>	ADP						
<input checked="" type="checkbox"/>	ATP						
<input checked="" type="checkbox"/>	AcCoA						