

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

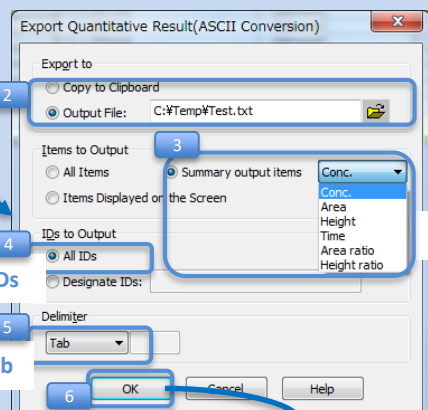
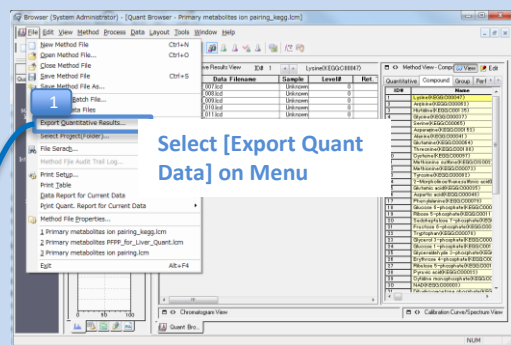


PREPARE INPUT DATA

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

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

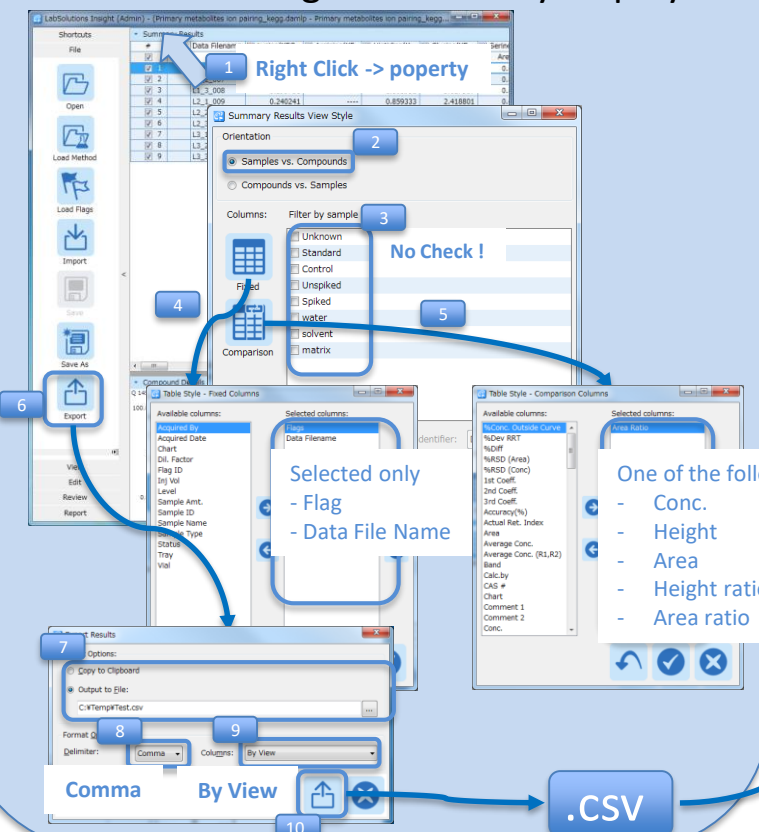
LabSolutions - Quant browser



Except Time

.txt

LabSolutions Insight - Summary display



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)

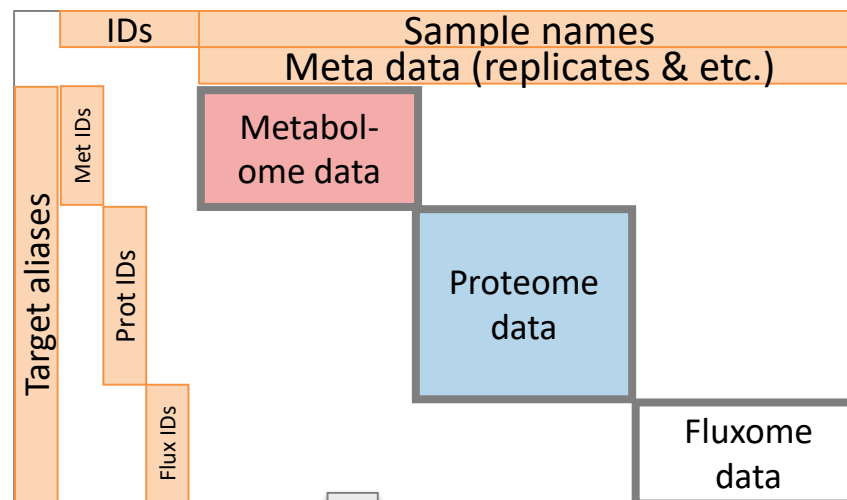


- Merge dataset
- Normalize data
- Average timecourse data
- Imputate data
- Select compounds

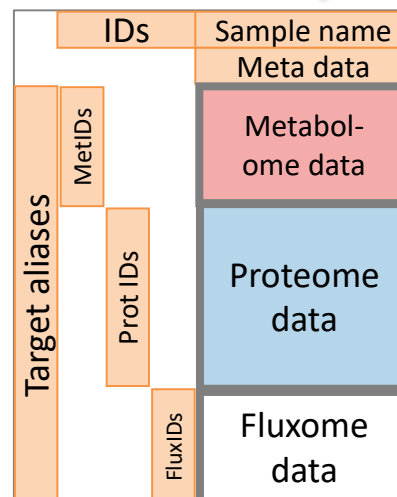
OUTPUT

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

(.szf)



Merge dataset





“Shimadzu MSdata Import” 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-S
(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	KTVPXQYAKDP...	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_1_m	S288C-S288C_2_m	S288C-S288C_3_m	pfi.Idelta	pfi.Idelta	pfi
(Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	0	0	0	0	0	0
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0	0	0	0	0	0
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	0	0	0	0	0	0
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	0	0	0	0	0	0
1	<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLSJ...	C00092	0.255	0.315	0.288	0.721	0.5	0.5
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPXQYAKDP...	C00117	0.007	0.01	0.008	0.017	0.5	0.5

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-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	KTVPXQYAKDP...	C00117	0.015777777777777777
3	<input checked="" type="checkbox"/>	EXP	48153	NGHKNAPVRF...	C00279	0.1321111111111111
4	<input checked="" type="checkbox"/>	SIP	18721	LCTUMKQJSD...	C00492	0.1162222222222222
5	<input checked="" type="checkbox"/>	PYR	32816	LCTONKANCYL...	C00822	0.8887777777777777
6	<input checked="" type="checkbox"/>	DHAP	16108	ONGACRATGOG...	C00111	0.0711111111111111
7	<input checked="" type="checkbox"/>	AMP	16027	UDHBCSSLTH...	C00920	0.0145555555555555
8	<input checked="" type="checkbox"/>	FBP	16905	JFYBEMDQGN...	C00344	0.3749888888888889
9	<input checked="" type="checkbox"/>	3PG-2PG	17035	C00187	C00631	0.1862222222222222
10	<input checked="" type="checkbox"/>	PEP	18021	DTBENJWJW...	C00874	0.0394444444444444
11	<input checked="" type="checkbox"/>	EPG	48929	BRSZFKFOLS...	C00445	0.0155555555555555
12	<input checked="" type="checkbox"/>	ADP	16761	JXWYTFMLZFF...	C00880	0.035
13	<input checked="" type="checkbox"/>	ATP	16422	ZKHQZCANR...	C00922	0.0241111111111111
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZPFCDC...	C00824	0.0208888888888889
15	<input checked="" type="checkbox"/>	FBP	61553	BOWGPAPYGO...	C00885	0.0877777777777777
16	<input checked="" type="checkbox"/>	uAP	17883	FZLZVUNMG...	C00231	0.0195555555555555
17	<input checked="" type="checkbox"/>	NAD	15848	BNWFJLJZEF...	C00993	0.0077777777777777
18	<input checked="" type="checkbox"/>	NAD	15848	BNWFJLJZEF...	C00993	0.1191111111111111
19	<input checked="" type="checkbox"/>	NADP	18089	JCLJNLUYWG...	C00886	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

A imported data table is displayed here

	select	Name	CHEBI	Inchi	kegg	S288C:S288C_1_mv	S288C:S288C_2_mv	S288C:S288C_3_mv	pkf1delta	pkf1c
(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	NGHMDNPXVRF...	C00279	0.046	0.053	0.047	0.263	0.263
4	<input checked="" type="checkbox"/>	S7P	15721	JDTUMPKOJBQ...	C05382	0.029	0.038	0.032	0.234	0.24
5	<input checked="" type="checkbox"/>	PYR	32816	LCTONWCANYU...	C00022	0.806	0.825	0.763	1.092	0.812
6	<input checked="" type="checkbox"/>	DHAP	16108	GNGACRATGGD...	C00111	0.042	0.081	0.068	0.054	0.041
7	<input checked="" type="checkbox"/>	AMP	16097	UIMBPSITTH...	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	ZSLZBFCDGIB...	C00024	0.028	0.045	0.024	0.043	0.031
15	<input checked="" type="checkbox"/>	F6P	61553	BGWGXPAFYGQ...	C00085	0.031	0.025	0.03	0.061	0.058
16	<input checked="" type="checkbox"/>	Xu5P			C00231	0.008	0.013	0.012	0.023	0.02
17	<input checked="" type="checkbox"/>	Ru5P	17363	FNZLKVNUWIPS...	C00199	0.002	0.005	0.005	0.012	0.008
18	<input checked="" type="checkbox"/>	NAD	15846	BAWFJGJGJIEF...	C00003	0.112	0.169	0.112	0.144	0.162
19	<input checked="" type="checkbox"/>	NADP	16008	YHVKIYBYW...	C00006	0.043	0.06	0.037	0.047	0.04



Data Processing

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

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

Shimadzu MS data Import

File(F) Data(D) Filter

View

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

☐ Show : 2 Rows ☐ Merge by Sample

☐ Hide ID Columns ☐ Avg. of timecourse

Output Style

☒ Table

☐ List

Select All Deselect All Deselect Columns Load Initial Data **Clear Data**

	select	Name	CHEBI	Inchi	kegg	S288C-S288C_1_m	S288C-S288C_2_m	S288C-S288C_3_m	pkf1delta	pkf1_r	pkf1_c
(Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	S288C	S288C	S288C	pkf1delta	pkf1_r	pkf1_c
(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						0.813	0.721	
2	<input checked="" type="checkbox"/>	R5P	52742						0.022	0.017	
3	<input checked="" type="checkbox"/>	E4P	48153						0.263	0.263	
4	<input checked="" type="checkbox"/>	S7P	15721	JDTUMPKOJBQ...	C00382	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	XPYBSMDXQFN...	C00354	5.428	5.214	4.981	1.916	1.755	
9	<input checked="" type="checkbox"/>	3PG+2PG	17835	C00197	C00631	0.164	0.225	0.17	0.201	0.206	
10	<input checked="" type="checkbox"/>	PEP	18021	DTBNBXWJWCW...	C00074	0.029	0.038	0.026	0.043	0.046	
11	<input checked="" type="checkbox"/>	6PG	48928	BIPSGZKFKXLS...	C00345	0.073	0.075	0.073	0.092	0.078	
12	<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY...	C00008	0.012	0.054	0.034	0.053	0.044	
13	<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW...	C00002	0.399	0.633	0.313	0.609	0.434	
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFDCINB...	C00024	0.028	0.045	0.024	0.043	0.031	
15	<input checked="" type="checkbox"/>	F6P	61553	BGWSXPAPYQG...	C00085	0.031	0.025	0.03	0.061	0.058	
16	<input checked="" type="checkbox"/>	Xu5P			C00231	0.008	0.013	0.012	0.023	0.02	
17	<input checked="" type="checkbox"/>	Ru5P	17363	FNZLKVNLMPS...	C00199	0.002	0.005	0.005	0.012	0.008	
18	<input checked="" type="checkbox"/>	NAD	15846	BAWFJGJZGIEF...	C00003	0.112	0.169	0.112	0.144	0.162	

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

Shimadzu MS data Import

File(F) Data(D) Filter

View

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

☐ Show : 2 Rows ☐ Merge by Sample

☐ Hide ID Columns ☐ Avg. of timecourse

Output Style

☒ Table

☐ List

Select All Deselect All Deselect Columns Load Initial Data **Clear Data**

	select	Name	CHEBI	Inchi	kegg	S288C-S288C_1_m	S288C-S288C_2_m	S288C-S288C_3_m	pkf1delta	pkf1_r	pkf1_c
--	--------	------	-------	-------	------	-----------------	-----------------	-----------------	-----------	--------	--------



Data Processing

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

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

Shimadzu MS data Import

File Data Filter

View

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

☐ Show : 2 Rows ☐ Merge by Sample

☐ Hide ID Columns ☐ Avg. of timecourse

Output Style

☒ Table ☐ List

Select All Deselect All Deselect Columns Load Initial Data Clear Data

	select	Name	CHEBI	Inchi	kegg	S288C	S288C	S288C	pkf Idelta
(Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	0	0	0	0
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0	0	0	0
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	0	0	0	0
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	0	0	0	0
1	<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLSJ...	C00092	0.255	0.315	0.288	0.813
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPXQYAKDP...	C00117	0.007	0.01	0.008	0.022
3	<input checked="" type="checkbox"/>	E4P				0.046	0.053	0.047	0.263
4	<input checked="" type="checkbox"/>	S7P				0.029	0.038	0.032	0.234
5	<input checked="" type="checkbox"/>	PYR				0.806	0.825	0.763	1.092
6	<input checked="" type="checkbox"/>	DHAP				0.042	0.081	0.068	0.054
7	<input checked="" type="checkbox"/>	AMP				0.023	0.017	0.01	0.015
8	<input checked="" type="checkbox"/>	FBP	16905	XPYBSMDXQFN...	C00354	5.428	5.214	4.981	1.916
9	<input checked="" type="checkbox"/>	3PG+2PG	17835	C00197	C00631	0.164	0.225	0.17	0.201
10	<input checked="" type="checkbox"/>	PEP	18021	DTENBXWJMCW...	C00074	0.029	0.038	0.026	0.043
11	<input checked="" type="checkbox"/>	6PG	48928	BIRSGZKFKOLS...	C00345	0.073	0.075	0.073	0.092
12	<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY...	C00008	0.012	0.054	0.034	0.053
13	<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW...	C00002	0.399	0.633	0.313	0.609
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFDCDINB...	C00024	0.028	0.045	0.024	0.043
15	<input checked="" type="checkbox"/>	F6P	61553	BGWGXPAFYGO...	C00085	0.031	0.025	0.03	0.061
16	<input checked="" type="checkbox"/>	Yu5P			C00231	0.008	0.013	0.012	0.023

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
(Sample Name)	<input checked="" type="checkbox"/>	(Sample Name)	*	*	*	0	0	0	0
(Sample ID)	<input checked="" type="checkbox"/>	(Sample ID)	*	*	*	0	0	0	0
(time course)	<input checked="" type="checkbox"/>	(time course)	*	*	*	1	1	1	2
(replicate)	<input checked="" type="checkbox"/>	(replicate)	*	*	*	0	0	0	0
1	<input checked="" type="checkbox"/>	G6P	4170	NBSCHQHZLSJ...	C00092	0.255	0.315	0.288	0.813
2	<input checked="" type="checkbox"/>	R5P	52742	KTVPXQYAKDP...	C00117	0.007	0.01	0.008	0.022
3	<input checked="" type="checkbox"/>	E4P	48153	NGHMDNPXVRF...	C00279	0.046	0.053	0.047	0.263
4	<input checked="" type="checkbox"/>	S7P	15721	JDTUMPKQJBQ...	C05382	0.029	0.038	0.032	0.234
5	<input checked="" type="checkbox"/>	PYR	32816	LOTONWCANYU...	C00022	0.806	0.825	0.763	1.092
6	<input checked="" type="checkbox"/>	DHAP	16108	GNGACRATGG...	C00111	0.042	0.081	0.068	0.054
7	<input checked="" type="checkbox"/>	AMP	16027	UOMBCCSLTHH...	C00020	0.023	0.017	0.01	0.015
8	<input checked="" type="checkbox"/>	FBP	16905	XPYBSMDXQFN...	C00354	5.428	5.214	4.981	1.916
9	<input checked="" type="checkbox"/>	3PG+2PG	17835	C00197	C00631	0.164	0.225	0.17	0.201
10	<input checked="" type="checkbox"/>	PEP	18021	DTENBXWJMCW...	C00074	0.029	0.038	0.026	0.043
11	<input checked="" type="checkbox"/>	6PG	48928	BIRSGZKFKOLS...	C00345	0.073	0.075	0.073	0.092
12	<input checked="" type="checkbox"/>	ADP	16761	XTWYTFMLZFPY...	C00008	0.012	0.054	0.034	0.053
13	<input checked="" type="checkbox"/>	ATP	15422	ZKHQWZAMYRW...	C00002	0.399	0.633	0.313	0.609
14	<input checked="" type="checkbox"/>	AcCoA	15351	ZSLZBFDCDINB...	C00024	0.028	0.045	0.024	0.043
15	<input checked="" type="checkbox"/>	F6P	61553	BGWGXPAFYGO...	C00085	0.031	0.025	0.03	0.061
16	<input checked="" type="checkbox"/>	Yu5P			C00231	0.008	0.013	0.012	0.023

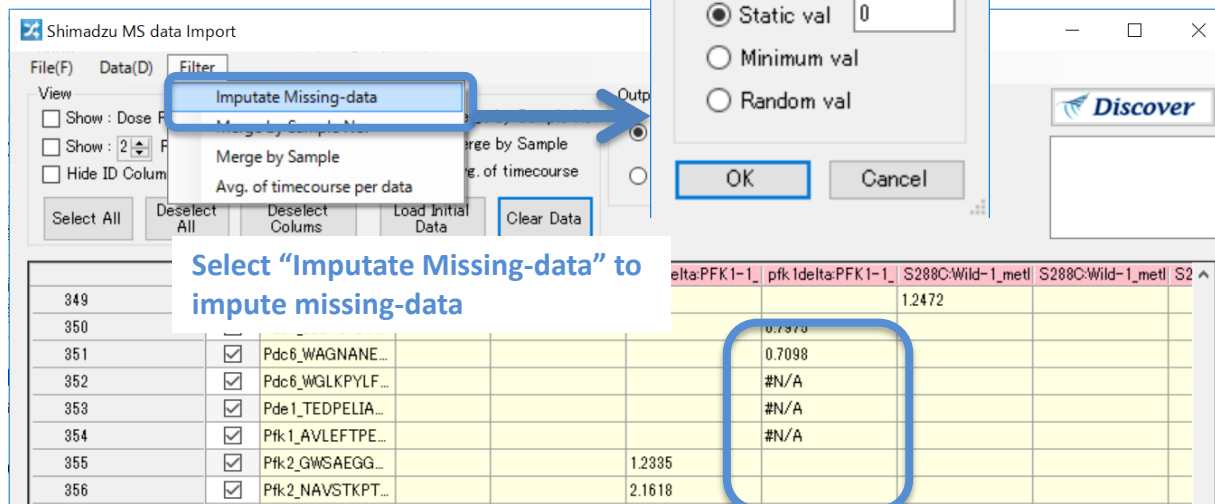


Data Processing

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

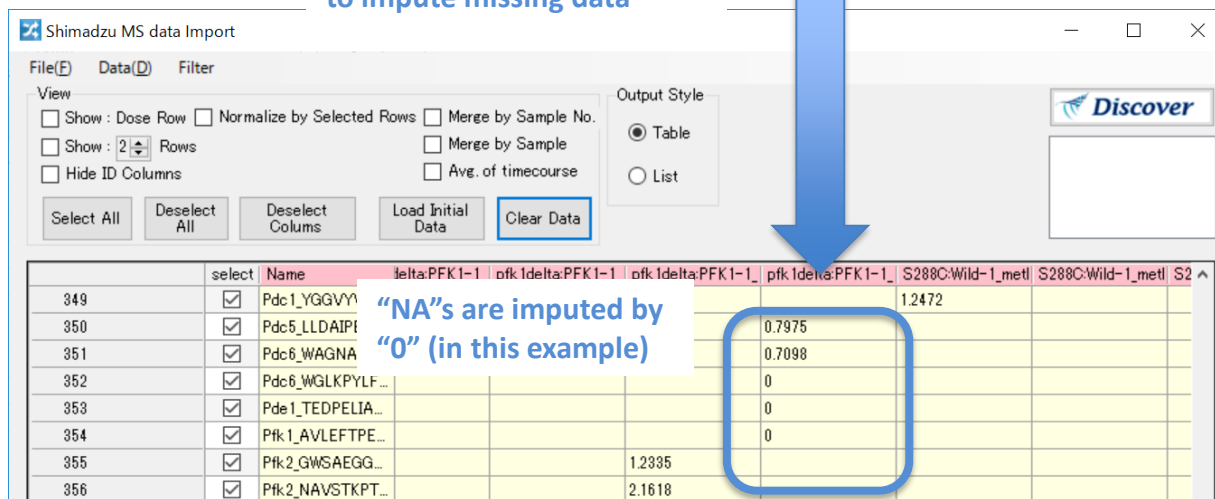
1. Select **"Impute Missing-data"** to impute missing-data (e.g., NA) in the imported omics data. By clicking the button, a window (see dialog ②) comes up.
2. **"All data"** and **"Selected"** indicate target data cells (all cells and selected cell respectively) to impute missing-data. **"Static val"**,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

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



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

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



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



Data Processing

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

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

Shimadzu MS data Import

File Data Filter

View

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

☐ Show : 2 Rows

☐ Hide ID Columns

Output Style

☐ Merge by Sample

☒ Avg. of timecourse

☒ Table

☐ List

Select All Deselect All Deselect Columns Load Initial Data Clear Data

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	0.763	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	0.886	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

Shimadzu MS data Import

File Data Filter

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Output Style

☐ Merge by Sample

☒ Avg. of timecourse

☒ Table

☐ List

Select All Deselect All Deselect Columns Load Initial Data Clear Data

Discover

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	0.833666666666...	0.256666666666...
2	R5P	52742	KTVPXQYAKDP...	C00117	0.008333333333...	0.021333333333...	0.017666666666...
3	E4P	48153	NGHMDNPXVRF...	C00279	0.048666666666...	0.291	0.056666666666...
4	S7P	15721	JDTUMPKOJBO...	C05382	0.033	0.262	0.056666666666...
5	PYR	32816	LCTONWCANYU...	C00022	0.798	0.994	0.874333333333...
6	DHAP	16108	GNACRATGGD...	C00111	0.063666666666...	0.056666666666...	0.093
7	AMP	16027	UDMBCSLTHH...	C00020	0.016666666666...	0.014	0.013
8	FBP	16905	XPYBSMDXQFN...	C00354	5.2076666666667	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	0.033333333333...	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	BGWGXFPAPYGO...	C00085	0.029666666666...	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	BAWFJGJGIEF...	C00003	0.131	0.144333333333...	0.082



Data Processing

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

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

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

Select All Deselect All Deselect Columns Load Initial Data Clear Data

Output Style

☐ Table

☐ List

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

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

Enter the “kegg” column



Shimadzu MS data Import

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Select All Deselect All Deselect Columns Load Initial Data Clear Data

Output Style

☐ Table

☒ List

Discover

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



OUTPUT

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

(.szf)

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

Click “**Discover**” to list up downstream analysis gadgets

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

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