Shimadzu
MSdata Import

2017 July

Shimadzu MSdata Import

What's New !

2017.07   v1.0.1   release
- [File] Add loadable text file format
  - LabSolutions : .txt file
  - LabSolutions Insight : .csv file

Release Note:
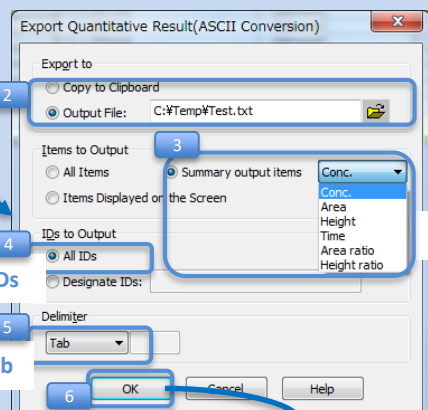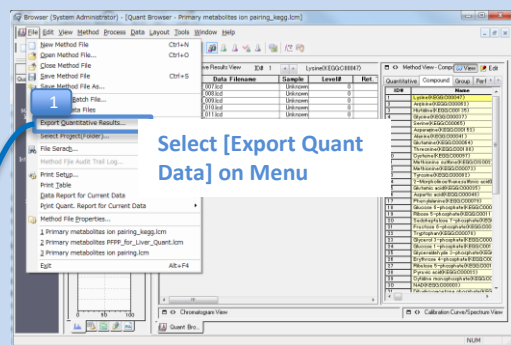2017.06   v1.0   release

Shimadzu MSdata Import

PREPARE INPUT DATA
- LabSolutions (.txt)
- LabSolutions Insight (.csv, .txt)

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

LabSolutions - Quant browser
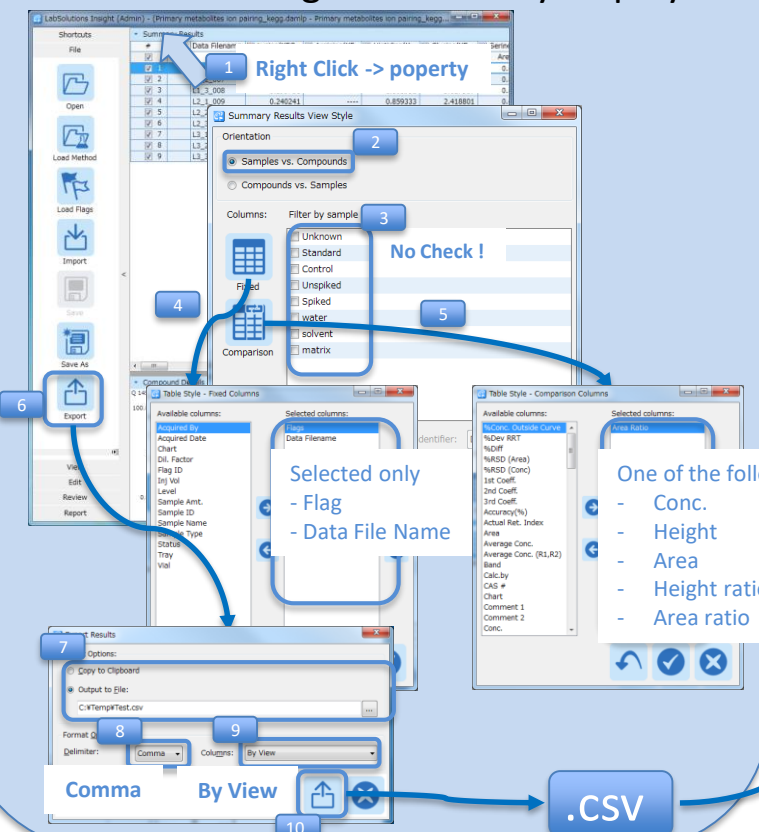
Select [Export Quant Data] on Menu

Except Time

All IDs

Tab

.txt

LabSolutions Insight - Summary display

Right Click -> poperty

No Check !

Selected only
- Flag
- Data File Name

One of the following
- Conc.
- Height
- Area
- Height ratio
- Area ratio

Comma   By View

.CSV

Shimadzu MSdata Import

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
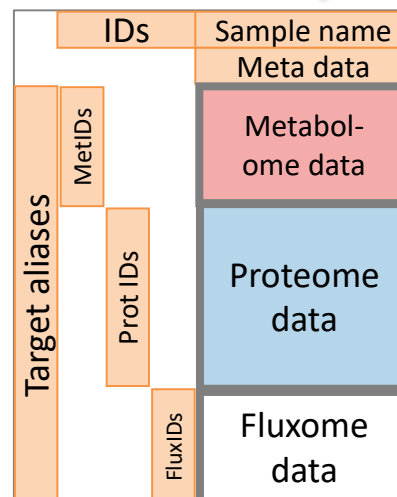- Imputate data
- Select compounds

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

(.szf)
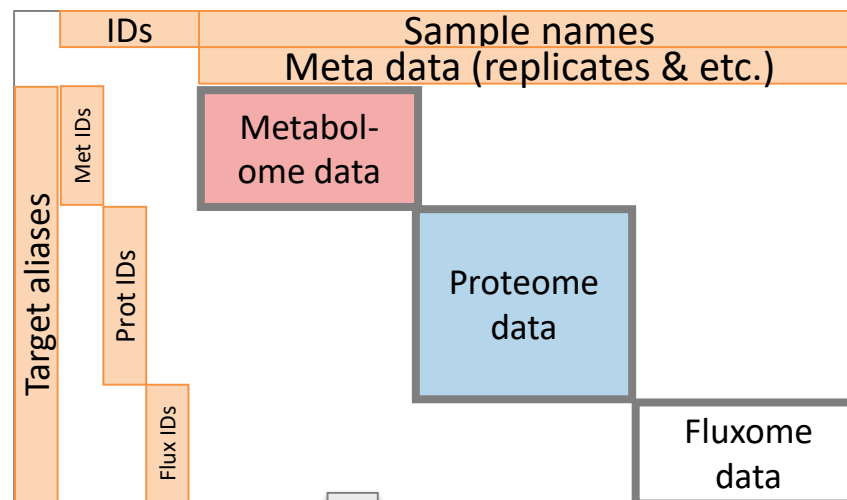
Merge dataset

Shimadzu MSdata Import

"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

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

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.

Click "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

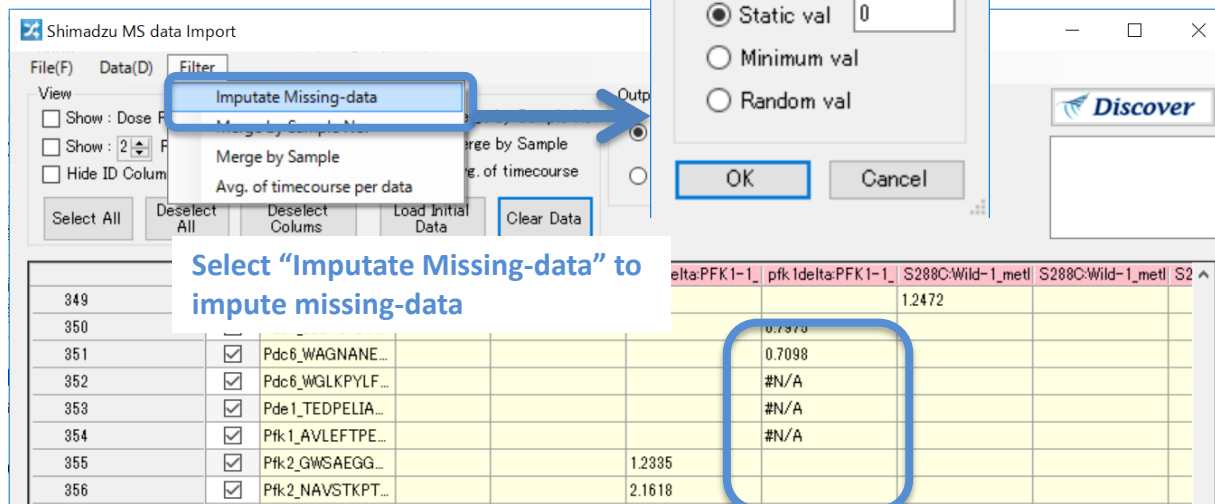1. Select cells to edit the data in the cells.

Shimadzu MSdata Import

Data Processing

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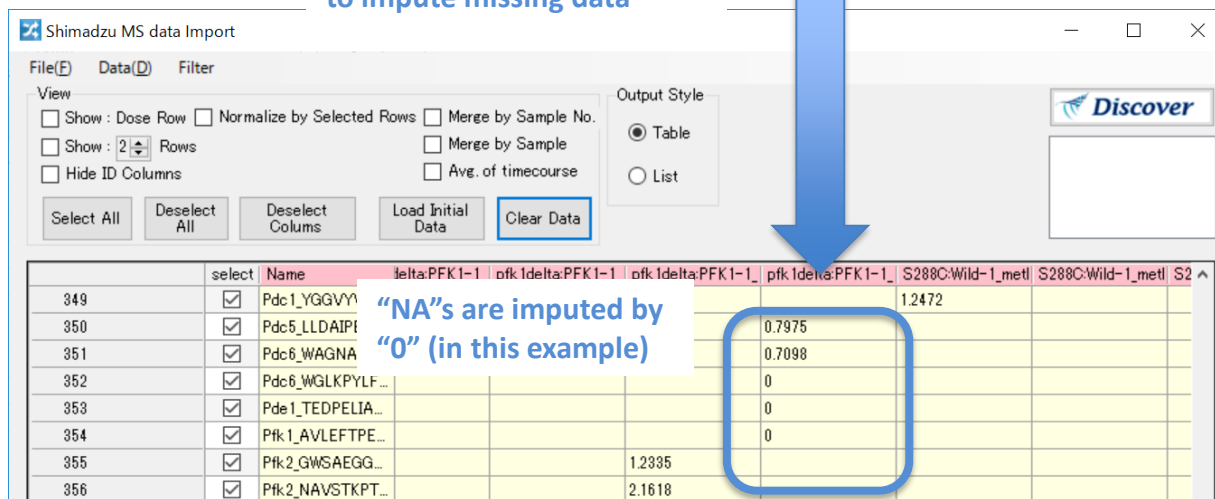- Merge dataset
- Select Output Style

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

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

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

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

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.

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

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.

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

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.

Click "Discover" to list up downstream analysis gadgets

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