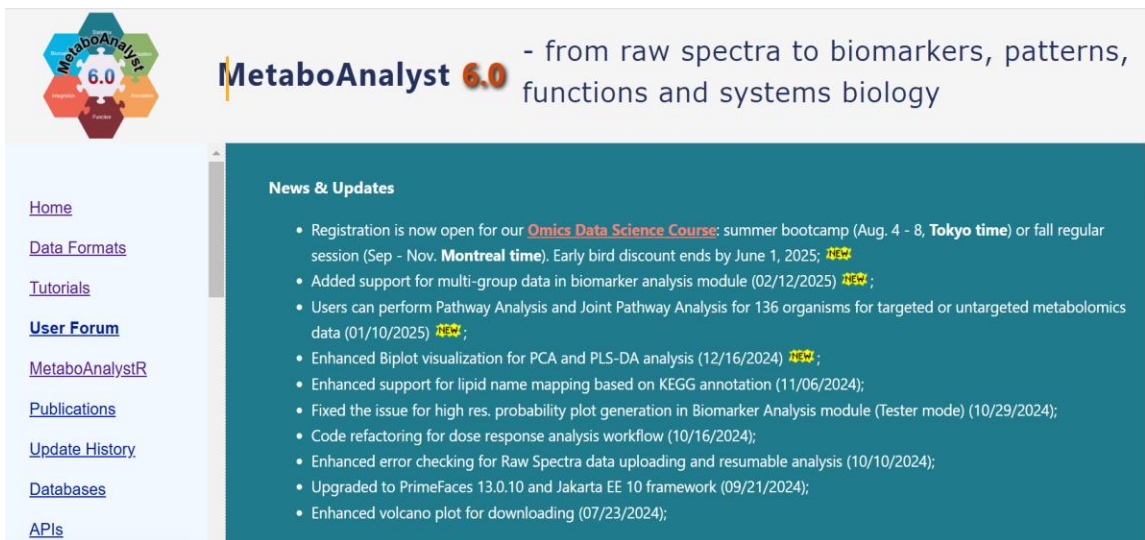


MetaboAnalyst

②「Data Formats」をクリックし、例えば「cow_diet.csv」をダウンロード

① <https://www.metaboanalyst.ca/> にアクセス

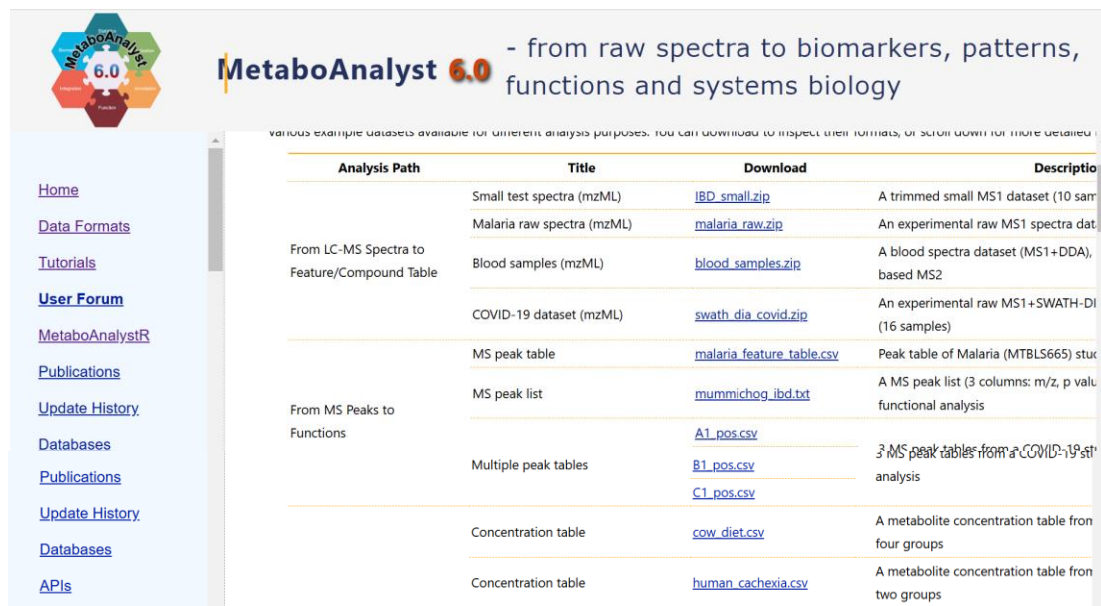


MetaboAnalyst 6.0 - from raw spectra to biomarkers, patterns, functions and systems biology

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News & Updates

- Registration is now open for our **Omics Data Science Course**: summer bootcamp (Aug. 4 - 8, **Tokyo time**) or fall regular session (Sep - Nov, **Montreal time**). Early bird discount ends by June 1, 2025; [NSF](#)
- Added support for multi-group data in biomarker analysis module (02/12/2025) [NSF](#);
- Users can perform Pathway Analysis and Joint Pathway Analysis for 136 organisms for targeted or untargeted metabolomics data (01/10/2025) [NSF](#);
- Enhanced Biplot visualization for PCA and PLS-DA analysis (12/16/2024) [NSF](#);
- Enhanced support for lipid name mapping based on KEGG annotation (11/06/2024);
- Fixed the issue for high res. probability plot generation in Biomarker Analysis module (Tester mode) (10/29/2024);
- Code refactoring for dose response analysis workflow (10/16/2024);
- Enhanced error checking for Raw Spectra data uploading and resumable analysis (10/10/2024);
- Upgraded to PrimeFaces 13.0.10 and Jakarta EE 10 framework (09/21/2024);
- Enhanced volcano plot for downloading (07/23/2024);



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various example datasets available for different analysis purposes. You can download to inspect their formats, or scroll down for more details.

Analysis Path	Title	Download	Description
From LC-MS Spectra to Feature/Compound Table	Small test spectra (mzML)	IBD_small.zip	A trimmed small MS1 dataset (10 samples)
	Malaria raw spectra (mzML)	malaria_raw.zip	An experimental raw MS1 spectra dataset
	Blood samples (mzML)	blood_samples.zip	A blood spectra dataset (MS1+DDA), based MS2
From MS Peaks to Functions	COVID-19 dataset (mzML)	swath_dia_covid.zip	An experimental raw MS1+SWATH-DIA (16 samples)
	MS peak table	malaria_feature_table.csv	Peak table of Malaria (MTBLS665) study
	MS peak list	mummichog_ibd.txt	A MS peak list (3 columns: m/z, p value, functional analysis)
	Multiple peak tables	A1_pos.csv B1_pos.csv C1_pos.csv	3 MS peak tables from a COVID-19 study analysis
	Concentration table	cow_diet.csv	A metabolite concentration table from four groups
Concentration table	human_cachexia.csv	A metabolite concentration table from two groups	



Click here to start

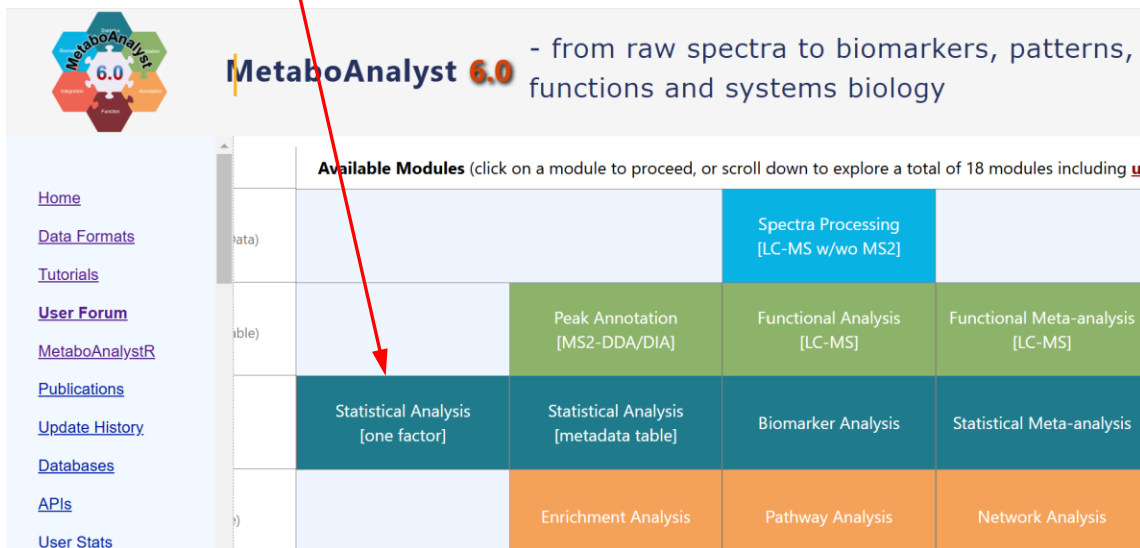
③ クリックしてスタート
→ 以下のポップアップで「Continue Analysis」をクリック

User Survey Request ×

Sorry for the inconvenience, please complete a brief (2~3 min) user survey to help keep the site funded. Thank you.

[Perform Survey](#) [Continue Analysis](#)

④ 「Statistical Analysis[one factor]」をクリック



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Available Modules (click on a module to proceed, or scroll down to explore a total of 18 modules including **un**)

(ata)		Spectra Processing [LC-MS w/wo MS2]		
(ible)	Peak Annotation [MS2-DDA/DIA]	Functional Analysis [LC-MS]	Functional Meta-analysis [LC-MS]	
	Statistical Analysis [one factor]	Statistical Analysis [metadata table]	Biomarker Analysis	Statistical Meta-analysis
)		Enrichment Analysis	Pathway Analysis	Network Analysis



⑤ Data Fileに②でダウンロードした「cow_diet.csv」を指定→Submit

Please upload your data

A plain text file (.txt or .csv):

濃度形式

Data Type: Concentrations Spectral bins Peak intensities

Format: Samples in rows (unpaired)

Data File: cow_diet.csv 10.5 KB

A compressed file (.zip):

Data Type: NMR peak list MS peak list

Data File:

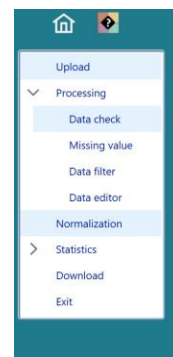
human_cachexia.csv 2025/02/27 11:55

cow_diet.csv 2025/02/27 11:33

大豆粉.MTW 2025/02/27 10:02



⑦「Normalize」をクリック→ OK表示→ Proceedクリック



Normalization Overview:

The normalization procedures are grouped into three categories. You can use one or combine them to achieve better results.

- Sample normalization is for general-purpose adjustment for systematic differences among samples;
- Data transformation applies a mathematical transformation on individual values themselves. A simple mathematical approach is used to deal with negative values in log and square root. Please search OmicsForum using "normalization #metaboanalyst" to find more information.
- Data scaling adjusts each variable/feature by a scaling factor computed based on the dispersion of the variable.

Sample normalization

- None
- Sample-specific normalization (i.e. weight, volume) Specify
- Normalization by sum
- Normalization by median

Data scaling

- None
- Mean centering (mean-centered only)
- Auto scaling (mean-centered and divided by the standard deviation of each variable)
- Pareto scaling (mean-centered and divided by the square root of the standard deviation of each variable)
- Range scaling (mean-centered and divided by the range of each variable)

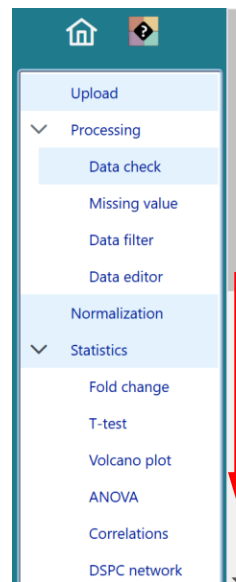


OK

You can click **View Result** button to view the effect, or **Proceed** button to analysis page!



⑧下方にスクロールして処理したい統計手法をクリック



Select an analysis path to explore :

Univariate Analysis

Fold Change Analysis T-tests Volcano plot

[One-way Analysis of Variance \(ANOVA\)](#)

[Correlation Heatmaps](#) [Pattern Search](#) [Correlation Networks \(DSPC\)](#)

Advanced Significance Analysis

[Significance Analysis of Microarray \(and Metabolites\) \(SAM\)](#)

Empirical Bayesian Analysis of Microarray (and Metabolites) (EBAM)

Chemometrics Analysis

[Principal Component Analysis \(PCA\)](#)

[Partial Least Squares - Discriminant Analysis \(PLS-DA\)](#)

[Sparse Partial Least Squares - Discriminant Analysis \(sPLS-DA\)](#)

Orthogonal Partial Least Squares - Discriminant Analysis (orthoPLS-DA)

This is mainly designed for better interpretation in comparison of two groups (control vs treatment). For multi-

Data Integrity Check:

- Checking sample names - spaces will be replaced with underscore, and special characters will be removed;
- Checking the class labels - at least three replicates are required in each class.
- The data (except class labels) must not contain non-numeric values.
- If the samples are paired, the pair labels must conform to the specified format.
- The presence of missing values or features with constant values (i.e. all zeros).

Data processing information:

Checking data content ...passed.
 Samples are in rows and features in columns
 The uploaded file is in comma separated values (.csv) format.
 The uploaded data file contains 39 (samples) by 47 (compounds) data matrix.
 Samples are not paired.
 4 groups were detected in samples.

Only English letters, numbers, underscore, hyphen and forward slash (/) are allowed.

Other special characters or punctuations (if any) will be stripped off.

All data values are numeric.

A total of 0 (0%) missing values were detected.

By default, missing values will be replaced by 1/5 of min positive values of their corresponding variables

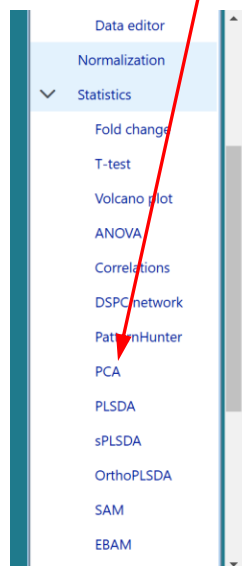
Click the **Proceed** button if you accept the default practice;

Or click the **Missing Values** button to use other methods.

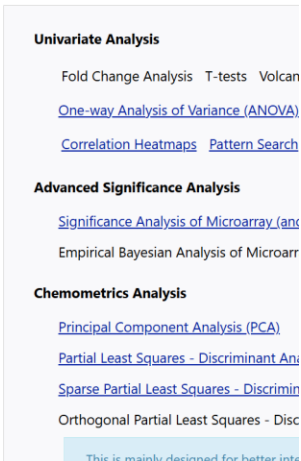
⑥ Proceedクリック



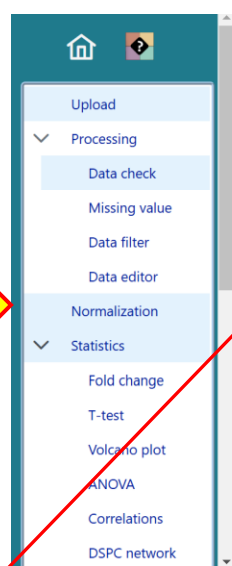
⑨PCA(主成分分析)をクリック



Select an analysis path to explore



⑩実行結果が表示→ 見たいグラフを選択



Principal Component Analysis (PCA)

