

# A simple session with MetaboAnalyst 3.0 (Nov. 2016)

*Perform statistical analysis using MetaboAnalyst on exported data from NMRProcFlow*

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## Data Export

A simple session with MetaboAnalyst 3.0



Processing Bucketing Data Export

### Data Type to Export:

- ☒ Data matrix
- ☐ Buckets table
- ☐ SNR matrix
- ☐ XLSX Workbook
- ☐ Spectral data
- ☐ Macro-Commands

### Export Format:

Comma Separator Value (CSV)

### Normalization Method:

Constant Sum Normalization

### SNR threshold:

3

### PPM range of the Reference:

### noisy PPM range:

10.5 10.2

Export Data Matrix

data\_NMRFRIM3-4.xlsx

Samplecode	Condition	Stage	B9_1272	B8_5408	B8_4573	B8_2825	B7_5855	B7_6635	B7_4512	B7_4362	B7_4224	B7_4090	B7_3957	B7_3834	B7_3711
F3-001	Control	J08	0.11523791	0.00581334	0.16150283	0.047086	0.09814524	0.09813412	0.01898936	0.03941068	0.04948976	0.02022299	0.00373634	0.02378087	0.02378087
F3-049	Control	J08	0.10384242	0.00835102	0.13585457	0.06159699	0.14618664	0.14036055	0.01539754	0.01692683	0.01200164	0.01717897	0.01085015	0.02315004	0.02315004
F3-097	Control	J08	0.09651629	0.00523615	0.17493857	0.06213409	0.16545419	0.18503065	0.02161687	0.0214187	0.02813971	0.02358135	0.01270131	0.02634738	0.02634738
F3-002	Shadow	J08	0.09611617	0.00458309	0.17093983	0.04593351	0.0781413	0.06906432	0.01626121	0.02980209	0.03109361	0.01965519	0.01404522	0.02284019	0.02284019
F3-050	Shadow	J08	0.12593911	0.01304445	0.13824284	0.05809637	0.14435492	0.13533937	0.03232633	0.01034411	0.01846426	0.02983426	0.02225713	0.03401898	0.03401898
F3-098	Shadow	J08	0.12360064	0.00724083	0.12777933	0.05951439	0.17228324	0.16153312	0.04384093	0.01533951	0.01755694	0.03644395	0.01806933	0.0401551	0.0401551
F3-013	Control	J15	0.05330992	0.00196927	0.13305672	0.0445001	0.0490723	0.04415489	0.01263968	0.03341843	0.04544959	0.02119349	0.01533574	0.02041401	0.02041401
F3-061	Control	J15	0.06667186	0.00552217	0.08759005	0.04733081	0.03781117	0.03933464	0.02078347	0.05830485	0.07758045	0.0348291	0.01933022	0.03107577	0.03107577
F3-109	Control	J15	0.07548592	0.0043433	0.08751526	0.04697576	0.05321745	0.05336447	0.00708144	0.0600623	0.08110833	0.03416974	0.01334663	0.03504505	0.03504505
F3-062	Shadow	J15	0.05700347	0.00229657	0.07625981	0.04703255	0.03478351	0.02437456	0.01564896	0.04840928	0.0614291	0.02940266	0.01571519	0.02557809	0.02557809
F3-110	Control	J15	0.08843008	0.00366854	0.11023306	0.01240016	0.04629357	0.0565123	0.02686256	0.03765864	0.046656	0.02004858	0.01410488	0.02813436	0.02813436
F3-025	Control	J15	0.04971968	0.00192048	0.07801866	0.02777739	0.05304738	0.02581476	0.00771899	0.05555394	0.06138559	0.03070073	0.01540366	0.02825725	0.02825725
F3-073	Control	J15	0.05267122	0.0042229	0.09108597	0.03208542	0.04221378	0.02215247	0.02931834	0.07019428	0.0875616	0.04830502	0.02846465	0.04251691	0.04251691
F3-121	Control	J28	0.04571739	0.00247732	0.06571802	0.04087093	0.01940316	0.01835539	0.01829224	0.06595428	0.11116443	0.04523421	0.02965821	0.04415303	0.04415303
F3-026	Shadow	J28	0.0418849	0.00111314	0.06341996	0.02773082	0.01097475	0.01296508	0.01251698	0.0412173	0.04200217	0.0241513	0.01693586	0.02228252	0.02228252
F3-074	Shadow	J28	0.05363533	0.00261704	0.07941371	0.02939763	0.0131065	0.02418532	0.01724451	0.06383088	0.10181302	0.04628110	0.02906383	0.04369965	0.04369965
F3-122	Shadow	J28	0.05738645	0.00203373	0.06136753	0.04243531	0.02371078	0.01953007	0.03795215	0.08552814	0.10944816	0.04547477	0.03542677	0.04118655	0.04118655
F3-037	Control	J35	0.05166236	0.04100089	0.05889308	0.09333538	0.0081829	0.00884584	0.03447293	0.07298427	0.08325465	0.03443659	0.02862395	0.03033902	0.03033902
F3-085	Control	J35	0.06717416	0.06835656	0.10970451	0.11024554	0.01595192	0.00927174	0.028818	0.07459614	0.07824352	0.02872809	0.04676672	0.03166967	0.03166967
F3-133	Control	J35	0.04319144	0.08358712	0.121372	0.13439019	0.00701626	0.01108497	0.02752508	0.09864951	0.11831952	0.04616909	0.05693713	0.04737119	0.04737119
F3-038	Shadow	J35	0.07895642	0.12345603	0.1278891	0.1784346	0.00541305	0.0076085	0.03272434	0.10715168	0.12007041	0.04038197	0.05594181	0.04416299	0.04416299
F3-086	Shadow	J35	0.07690517	0.09031835	0.12895566	0.14985144	0.01430116	0.00886306	0.01626272	0.06070653	0.07374108	0.02860104	0.05225686	0.02533339	0.02533339
F3-134	Shadow	J35	0.05143253	0.1055730	0.12400084	0.14763796	0.01646724	0.00440921	0.03305417	0.11258537	0.12189743	0.04185418	0.04906765	0.04550948	0.04550948
F4-001	Control	J08	0.1230095	0.0089157	0.16097331	0.05711378	0.14520576	0.16760372	0.03105041	0.03127852	0.03201556	0.02952918	0.02039009	0.03377415	0.03377415

Note that the embedded factors in the file come from the file of the samples provided at the data loading step

## Data Preparation

A simple session with MetaboAnalyst 3.0



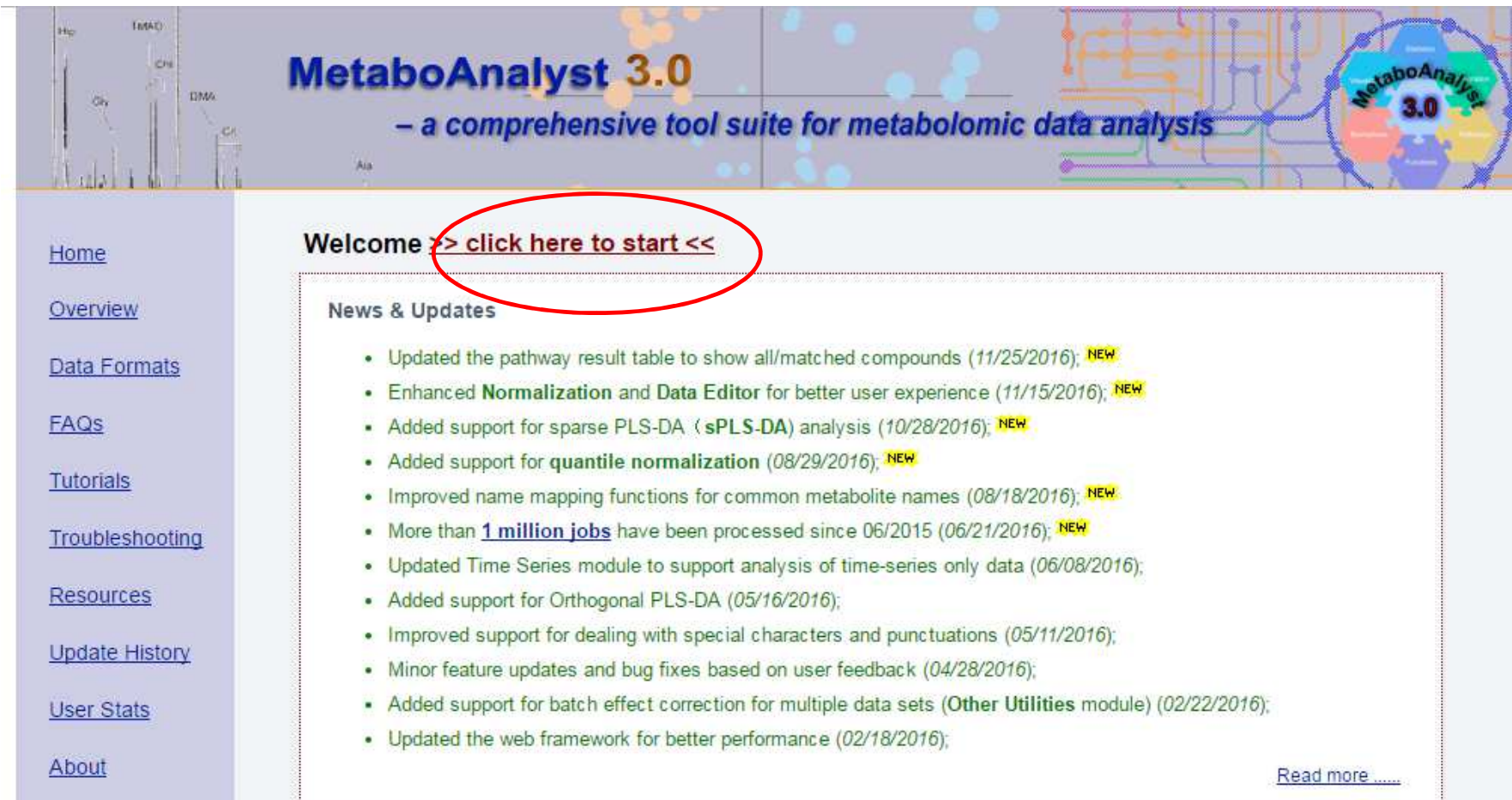
data\_NMRFRIM3-4\_2.csv

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	
1	Samplecode	Stage	B9_1272	B8_5408	B8_4573	B8_2825	B7_6956	B7_6635	B7_4512	B7_4362	B7_4224	B7_4090	B7_3957	B7_3834	B7_3439	B7_
2	F3-001	J08	0.11928791	0.00581534	0.16160283	0.047086	0.09814824	0.09813412	0.01898936	0.03941068	0.04948976	0.02022299	0.00373654	0.02378087	0.00837606	0.0
3	F3-049	J08	0.10384242	0.00835102	0.13589457	0.06159699	0.14618664	0.14036055	0.01539754	0.01692683	0.01200164	0.01717897	0.01085015	0.02315004	0.01097418	0.0
4	F3-097	J08	0.09651629	0.00623615	0.17493857	0.06213409	0.16545419	0.18503065	0.02161687	0.0214187	0.02813971	0.02358135	0.01270131	0.02834738	0.02033443	0.0
5	F3-002	J08	0.09611617	0.0045809	0.17093983	0.04593351	0.0781413	0.06906432	0.01626121	0.02980209	0.03109361	0.01965519	0.01404522	0.02284019	0.02623223	0.0
6	F3-050	J08	0.12598911	0.01304445	0.13824284	0.05809637	0.14435492	0.13533937	0.03232633	0.01034411	0.01846426	0.02983426	0.02225713	0.03401898	0.0151	0.0
7	F3-098	J08	0.12360064	0.00724083	0.12727933	0.05951439	0.17228824	0.16153312	0.04384093	0.01533951	0.01755694	0.03644395	0.01806933	0.0301551	0.01712958	0.0
8	F3-013	J15	0.05330992	0.00196927	0.13305672	0.0445001	0.0490723	0.04415489	0.01263968	0.03341843	0.04544959	0.02119349	0.01533574	0.02041401	0.03504713	0
9	F3-061	J15	0.06667186	0.00552217	0.08759005	0.04733081	0.03781117	0.03933464	0.02078347	0.05830485	0.07758045	0.0348291	0.01933022	0.03107577	0.03944734	0.0
10	F3-109	J15	0.07548592	0.0043453	0.08763526	0.04697576	0.05321745	0.05536447	0.00768144	0.0600623	0.08110839	0.03416974	0.01394663	0.03504505	0.03584766	0.0
11	F3-062	J15	0.05708147	0.00229657	0.07625981	0.04708255	0.03478851	0.02437456	0.01564896	0.04840928	0.0614291	0.02940266	0.01571519	0.02557809	0.03206315	0.0
12	F3-110	J15	0.08843008	0.00366854	0.11023306	0.04240016	0.04629357	0.0565123	0.02686256	0.03765864	0.046656	0.02004858	0.01410488	0.02813436	0.03500409	0.0
13	F3-025	J28	0.04971968	0.00192048	0.07801866	0.02777739	0.05304738	0.02581476	0.00771899	0.05553394	0.06138559	0.03070073	0.01540366	0.02825725	0.03624349	0.0
14	F3-073	J28	0.05267122	0.0042229	0.09108597	0.03208542	0.04221378	0.02215247	0.02931834	0.07019428	0.0875616	0.04830502	0.02846465	0.04251691	0.05215179	0.0
15	F3-121	J28	0.04971739	0.00247732	0.06571802	0.04087093	0.01940916	0.01839539	0.01829224	0.08595428	0.11116443	0.04523421	0.02985821	0.04415303	0.06111397	0.0
16	F3-026	J28	0.0418849	0.00111314	0.06341996	0.02779082	0.01097475	0.01296508	0.01251698	0.0412173	0.04200217	0.0241513	0.01693586	0.02228252	0.0354456	0.0
17	F3-074	J28	0.05363533	0.00261704	0.07941371	0.02939763	0.0131005	0.02418532	0.01724451	0.08383088	0.10181302	0.04628116	0.02906383	0.04369965	0.0661782	0.0
18	F3-122	J28	0.05738645	0.00203373	0.06196753	0.04248931	0.02371078	0.01953007	0.03795215	0.08552814	0.10944816	0.04647477	0.03542677	0.04118655	0.05864323	0.0
19	F3-037	J55	0.05166236	0.04100089	0.05889308	0.09333538	0.0081629	0.00884594	0.03447293	0.07293427	0.08325465	0.03443659	0.02862395	0.03033902	0.06994577	0.0
20	F3-085	J55	0.06712416	0.06835656	0.10920451	0.11024554	0.01595192	0.00922174	0.028818	0.07459614	0.07824352	0.02872809	0.04676672	0.03166962	0.06479155	0.0
21	F3-133	J55	0.04319144	0.08858712	0.121372	0.13439019	0.00701626	0.01108497	0.02752508	0.09864951	0.11831952	0.04616909	0.05693713	0.04737119	0.08907863	0.1
22	F3-038	J55	0.07895642	0.12345603	0.1278891	0.1784346	0.00541609	0.0076085	0.03272434	0.10715168	0.12007041	0.04038197	0.05594181	0.04416299	0.09458832	0.1
23	F3-086	J55	0.07690517	0.09031835	0.12899566	0.14985144	0.01430116	0.00886306	0.01626272	0.06070653	0.07374108	0.02860104	0.05225686	0.02533339	0.06451098	0.0
24	F3-134	J55	0.05143253	0.1055738	0.12400084	0.14763796	0.01646724	0.00440921	0.03385417	0.11258537	0.12189743	0.04185418	0.04906765	0.04950948	0.09579577	0.1
25	F4-001	J08	0.1230095	0.0089157	0.16097331	0.05711378	0.14520676	0.16760372	0.03105041	0.03127852	0.03201556	0.02952918	0.02039009	0.0337445	0.0251974	0.0
26	F4-009	J08	0.11805509	0.00993319	0.13889897	0.06237673	0.18644481	0.19322004	0.03153431	0.01269749	0.01392514	0.02890996	0.01090846	0.02709195	0.01678326	0.0
27	F4-065	J08	0.12751207	0.01224396	0.18111566	0.06507097	0.19123611	0.20620128	0.03532757	0.02819599	0.02656758	0.0267845	0.00161957	0.03110134	0.02248895	0.0
28	F4-005	J08	0.1521199	0.01065064	0.17468177	0.0523189	0.17477434	0.17434213	0.03837588	0.01809864	0.01769046	0.03640613	0.00352328	0.03113042	0.0141827	0.0
29	F4-069	J08	0.1213209	0.00979531	0.17288233	0.06183334	0.1343833	0.13361881	0.02614444	0.01241255	0.01158081	0.02226617	0.0023696	0.02982702	0.00378345	0.0
30	F4-037	J08	0.1463389	0.01302185	0.15087042	0.06193528	0.16628003	0.1734933	0.03825461	0.01474942	0.01645257	0.02830375	0.01310123	0.03292873	0.00387564	0.0
31	F4-017	J15	0.09974281	0.00592903	0.17961045	0.05311973	0.07853111	0.10013264	0.01403137	0.00769877	0.01132274	0.00369697	0.00665805	0.02183731	0.0068504	0.0



We keep only the "Stage" column as factor groups, given that MetaboAnalyst seems to accept only one factor.

<http://www.metaboanalyst.ca>



The screenshot shows the MetaboAnalyst 3.0 website. The header features a banner with the text "MetaboAnalyst 3.0 – a comprehensive tool suite for metabolomic data analysis" and a circular logo with the number 3.0. A left sidebar contains navigation links: Home, Overview, Data Formats, FAQs, Tutorials, Troubleshooting, Resources, Update History, User Stats, and About. The main content area displays a "Welcome" message with a red circle around the link "> click here to start <<". Below this is a "News & Updates" section with a list of updates, each dated and marked as "NEW". A "Read more" link is at the bottom right of the news section.

**MetaboAnalyst 3.0**  
– a comprehensive tool suite for metabolomic data analysis

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Welcome [> click here to start <<](#)

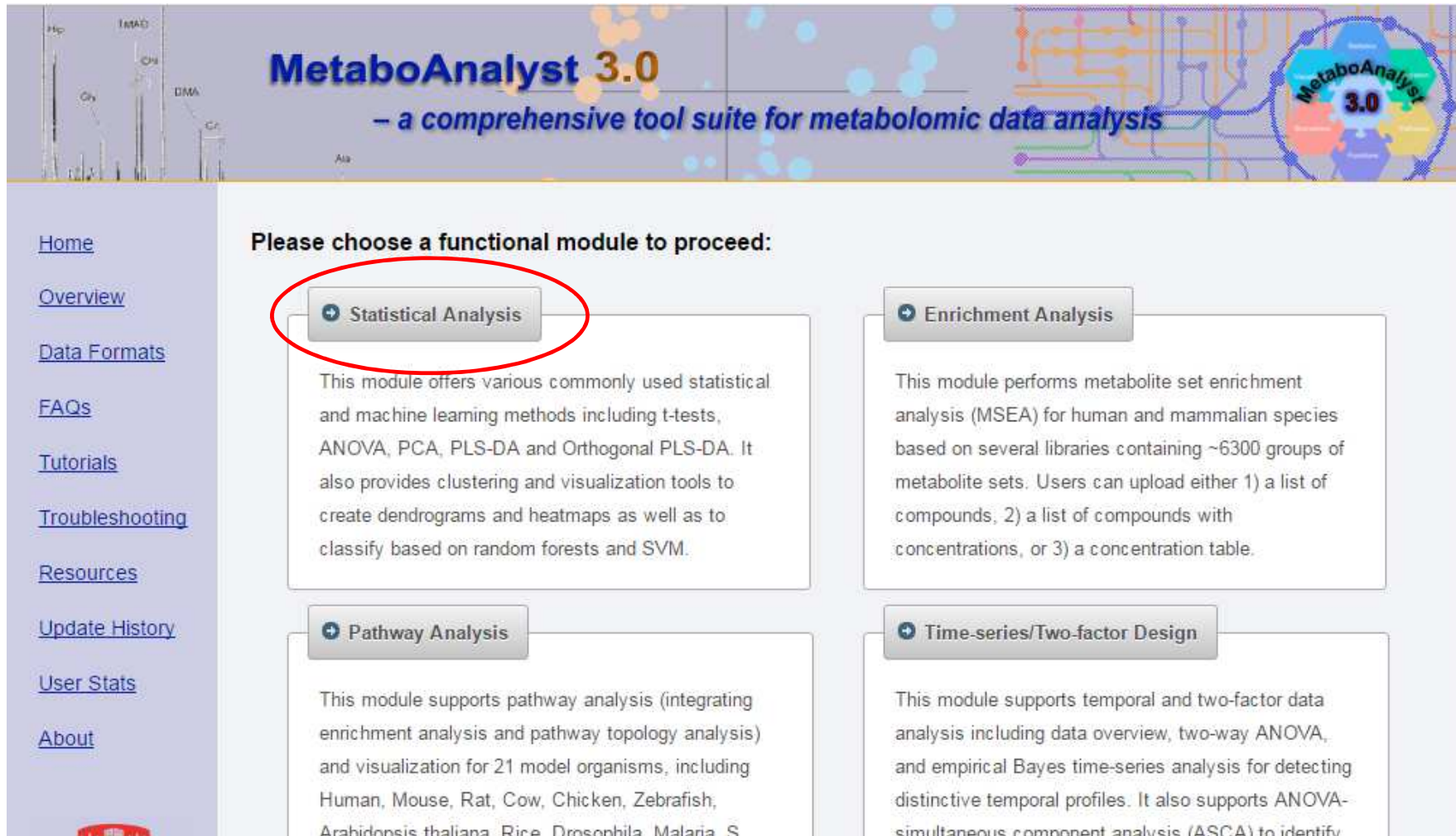
**News & Updates**

- Updated the pathway result table to show all/matched compounds (11/25/2016); **NEW**
- Enhanced **Normalization** and **Data Editor** for better user experience (11/15/2016); **NEW**
- Added support for sparse PLS-DA ( **sPLS-DA**) analysis (10/28/2016); **NEW**
- Added support for **quantile normalization** (08/29/2016); **NEW**
- Improved name mapping functions for common metabolite names (08/18/2016); **NEW**
- More than **1 million jobs** have been processed since 06/2015 (06/21/2016); **NEW**
- Updated Time Series module to support analysis of time-series only data (06/08/2016);
- Added support for Orthogonal PLS-DA (05/16/2016);
- Improved support for dealing with special characters and punctuations (05/11/2016);
- Minor feature updates and bug fixes based on user feedback (04/28/2016);
- Added support for batch effect correction for multiple data sets (**Other Utilities** module) (02/22/2016);
- Updated the web framework for better performance (02/18/2016);

[Read more .....](#)



## A simple session with MetaboAnalyst 3.0



The image shows the MetaboAnalyst 3.0 web interface. At the top, there is a header with the title "MetaboAnalyst 3.0" and the subtitle "– a comprehensive tool suite for metabolomic data analysis". The header also features a chromatogram on the left and a network diagram on the right. Below the header, there is a sidebar on the left with navigation links: Home, Overview, Data Formats, FAQs, Tutorials, Troubleshooting, Resources, Update History, User Stats, and About. The main content area is titled "Please choose a functional module to proceed:". There are four modules displayed in a 2x2 grid, each with a button and a description. The "Statistical Analysis" button is circled in red. The modules are: Statistical Analysis, Enrichment Analysis, Pathway Analysis, and Time-series/Two-factor Design.

**MetaboAnalyst 3.0**  
– a comprehensive tool suite for metabolomic data analysis

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**Please choose a functional module to proceed:**

- Statistical Analysis**  
This module offers various commonly used statistical and machine learning methods including t-tests, ANOVA, PCA, PLS-DA and Orthogonal PLS-DA. It also provides clustering and visualization tools to create dendrograms and heatmaps as well as to classify based on random forests and SVM.
- Enrichment Analysis**  
This module performs metabolite set enrichment analysis (MSEA) for human and mammalian species based on several libraries containing ~6300 groups of metabolite sets. Users can upload either 1) a list of compounds, 2) a list of compounds with concentrations, or 3) a concentration table.
- Pathway Analysis**  
This module supports pathway analysis (integrating enrichment analysis and pathway topology analysis) and visualization for 21 model organisms, including Human, Mouse, Rat, Cow, Chicken, Zebrafish, Arabidopsis thaliana, Rice, Drosophila, Malaria, S.
- Time-series/Two-factor Design**  
This module supports temporal and two-factor data analysis including data overview, two-way ANOVA, and empirical Bayes time-series analysis for detecting distinctive temporal profiles. It also supports ANOVA-simultaneous component analysis (ASCA) to identify

## A simple session with MetaboAnalyst 3.0

**MetaboAnalyst 3.0**  
– a comprehensive tool suite for metabolomic data analysis

**1) Upload your data**

Tab-delimited text (.txt) or **comma-separated values (.csv) file:**

**Data Type:** ☒ Concentrations ☐ Spectral bins ☐ Peak intensity table

**Format:** Samples in rows (unpaired)

**Data File:** Choose File data\_NMRF...3-4\_2.csv

**Submit**

**Zipped Files (.zip) :**

**Data Type:** ☒ NMR peak list ☐ MS peak list ☐ MS spectra

**Data File:** Choose File No file chosen

**Pair File:** Choose File No file chosen

**Submit**

**NMRProcFlow**

data\_NMRFRIM3-4\_2.csv

The interface shows the 'Upload your data' step. A blue arrow points to the '1) Upload your data' section. A red circle highlights the 'comma-separated values (.csv) file:' text. Another red circle highlights the 'Submit' button for the CSV upload. A blue arrow points from the 'data\_NMRF...3-4\_2.csv' file name to the 'data\_NMRFRIM3-4\_2.csv' file name in the NMRProcFlow section.

**Data Integrity Check:**

1. Checking the class labels - at least three replicates are required in each class.
2. If the samples are paired, the pair labels must conform to the specified format.
3. The data (except class labels) must not contain non-numeric values.
4. 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 43 (samples) by 357 (compounds) data matrix.

4 groups were detected in samples.

Samples are not paired.

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, these values will be replaced by a small value.



Click **Skip** button if you accept the default practice




Or click **Missing value imputation** to use other methods

**Missing value estimation** **Skip**

OK




  

  
 Processing
 

- Pre-process
- 
- Missing value
- 
- Data editor
- Image options
- 

Statistics
 

- Download
- Exit

## Data Filtering:


The purpose of the data filtering is to identify and remove variables that are unlikely to be of use when modeling the data. No phenotype information are used in the filtering process, so the result can be used with any downstream analysis. This step is strongly recommended for untargeted metabolomics datasets (i.e. spectral binning data, peak lists) with large number of variables, many of them are from baseline noises. Filtering can usually improve the results. For details, please refer to the paper by [Hackstadt, et al.](#)

Non-informative variables can be characterized in two groups: variables of **very small values** (close to baseline or detection limit) - these variables can be detected using mean or median; variables that are **near-constant values** throughout the experiment conditions (housekeeping or homeostasis) - these variables can be detected using standard deviation (SD); or the robust estimate such as interquartile range (IQR). The relative standard deviation ( $RSD = SD/mean$ ) is another useful variance measure independent of the mean. The following empirical rules are applied during data filtering:

- **Less than 250 variables:** 5% will be filtered;
- **Between 250 - 500 variables:** 10% will be filtered;
- **Between 500 - 1000 variables:** 25% will be filtered;
- **Over 1000 variables:** 40% will be filtered;

Please note, in order to reduce the computational burden to the server, the **None** option is only for less than 2000 features. Over that, if you choose None, the IQR filter will still be applied. In addition, the maximum allowed number of variables is 5000. If over 5000 variables were left after filtering, only the top 5000 will be used in the subsequent analysis.

☐ Interquartile range (IQR)
 ☐ Standard deviation (SD)
 ☐ Median absolute deviation (MAD)
 ☐ Relative standard deviation ( $RSD = SD/mean$ )
 ☐ Non-parametric relative standard deviation ( $MAD/median$ )
 ☐ Mean intensity value
 ☐ Median intensity value
 ☒ None (less than 2000 features)





**Normalization overview:**

The normalization procedures are grouped into three categories. The sample normalization allows general-purpose adjustment for differences among your sample; data transformation and scaling are two different approaches to make individual features more comparable. You can use one or combine them to achieve better results.

**Sample normalization**

- ☒ None
- ☐ Sample-specific normalization (i.e. weight, volume) [Click here to specify](#)
- ☐ Normalization by sum
- ☐ Normalization by median
- ☐ Normalization by a specific reference sample
- ☐ Normalization by a pooled sample from group
- ☐ Normalization by reference feature
- ☐ Quantile normalization

**Data transformation**

- ☒ None
- ☐ Log transformation (generalized logarithm transformation or glog)
- ☐ Cube root transformation (take cube root of data values)

**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 standard deviation of each variable)
- ☐ Range scaling (mean-centered and divided by the range of each variable)

**Normalization Method:**

Constant Sum Normalization

**SNR threshold:**

3

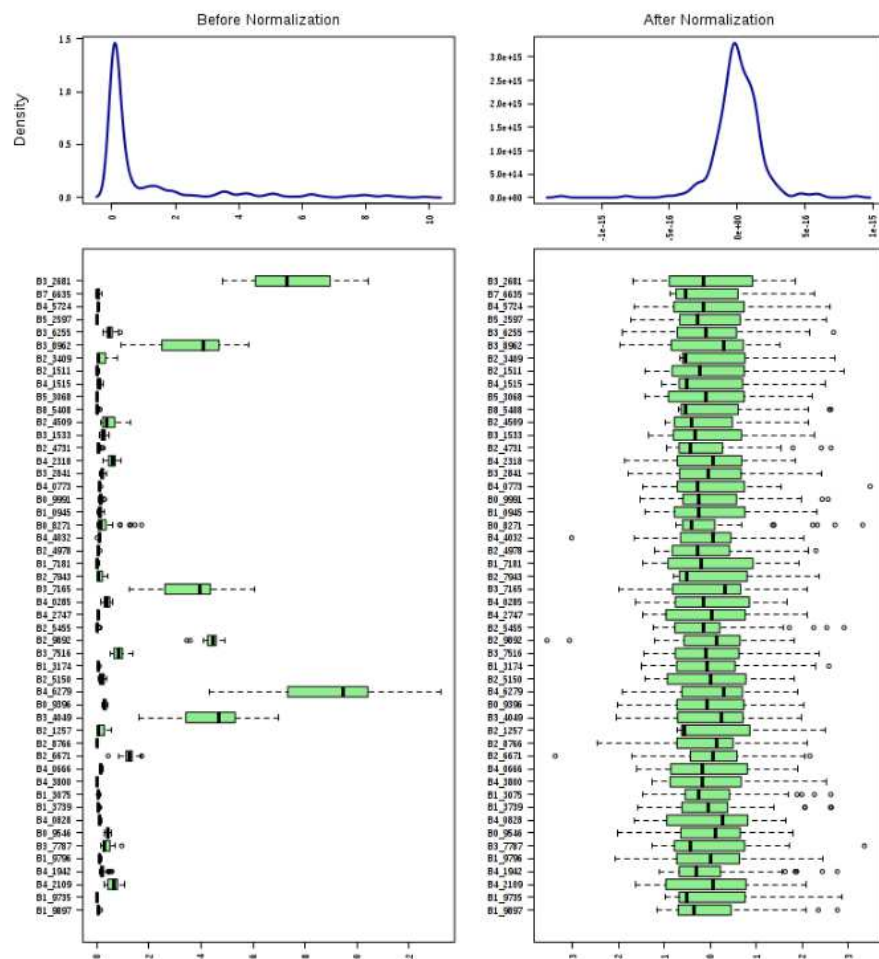
**Buttons:** Upload, Processing, Pre-process, Data check, Missing value, Data filter, Data editor, Image options, Normalization, Statistics, Download, Exit, Normalize, View Result, Proceed

**Note:**  
These choices are a direct consequence of the parameter values chosen during the data export step in NMRProcFlow

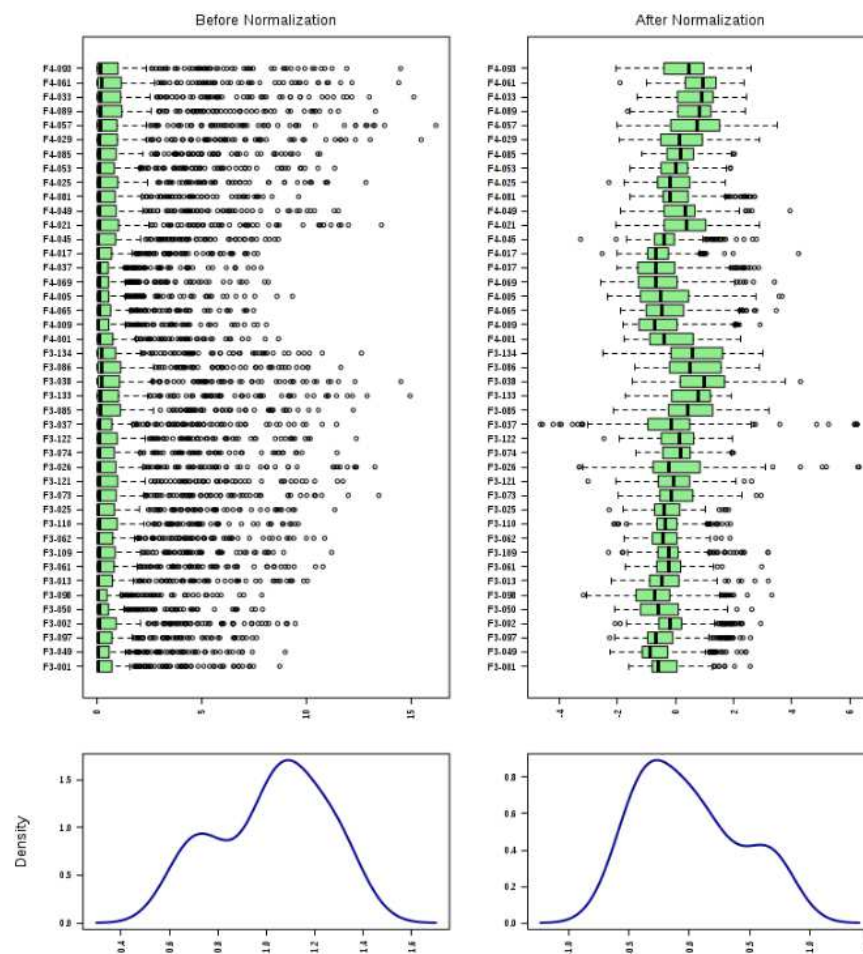
**OK**  
You can click **View Result** button to view the effect, or **Proceed** button to analysis page!

# A simple session with MetaboAnalyst 3.0

Feature View Sample View

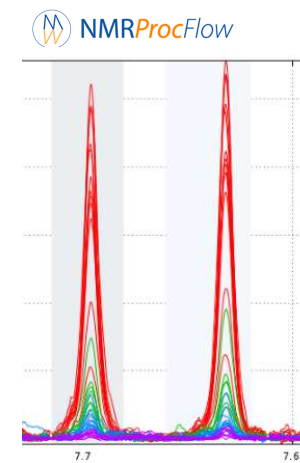
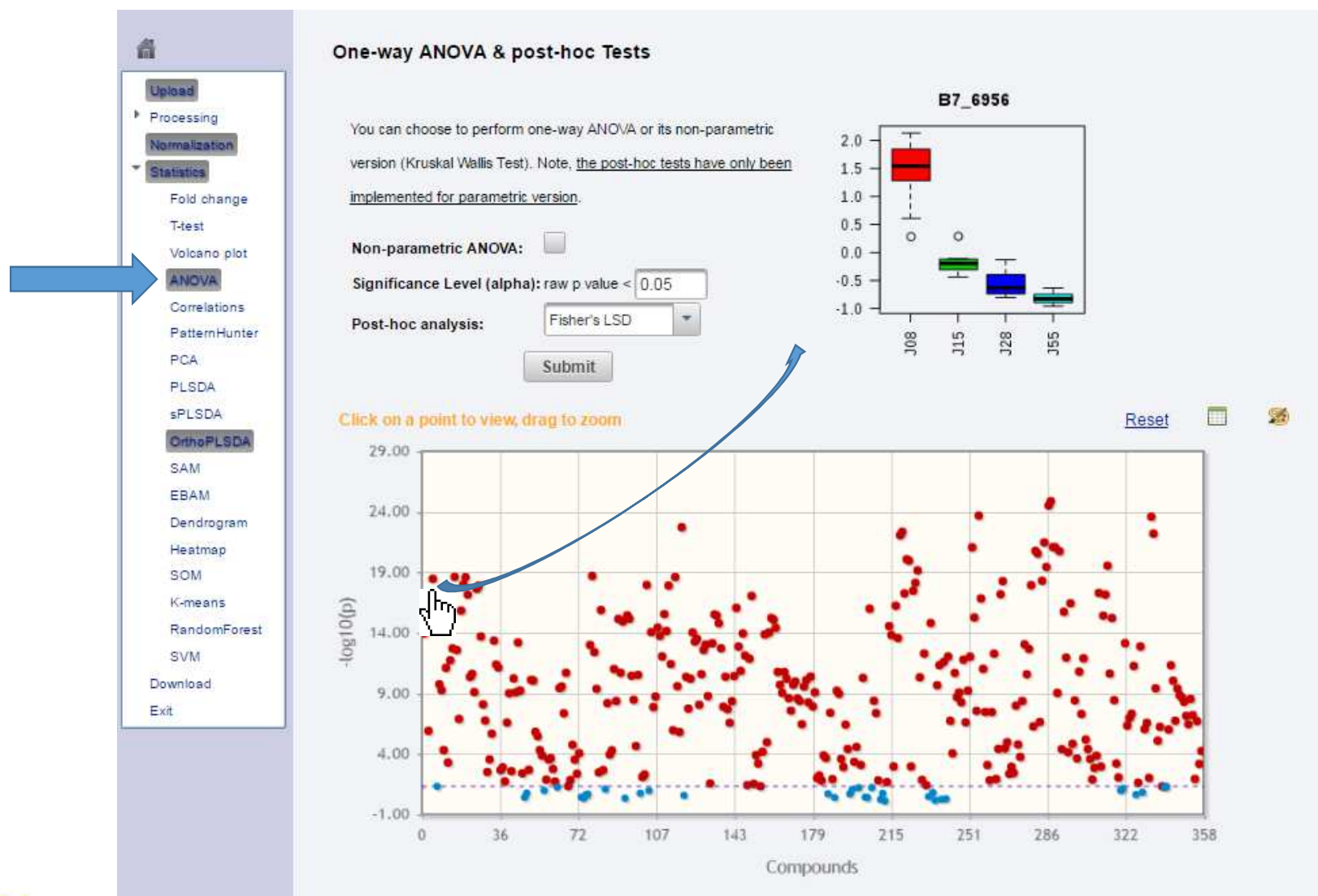


Feature View Sample View



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





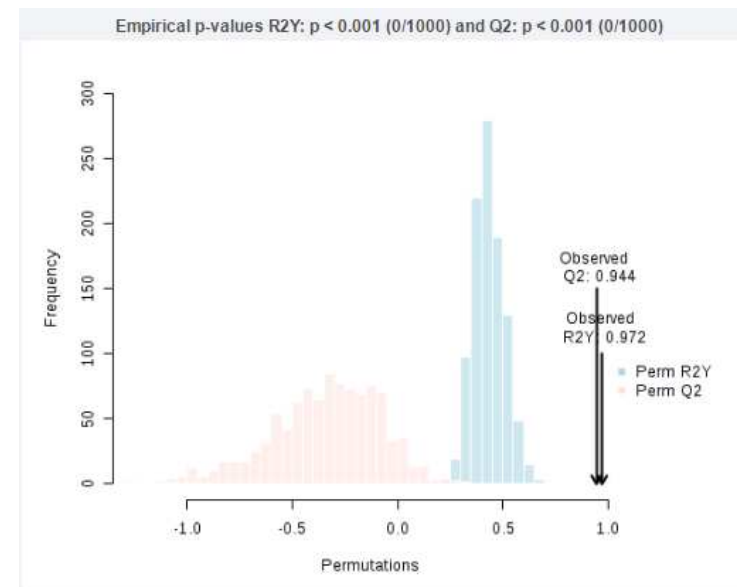
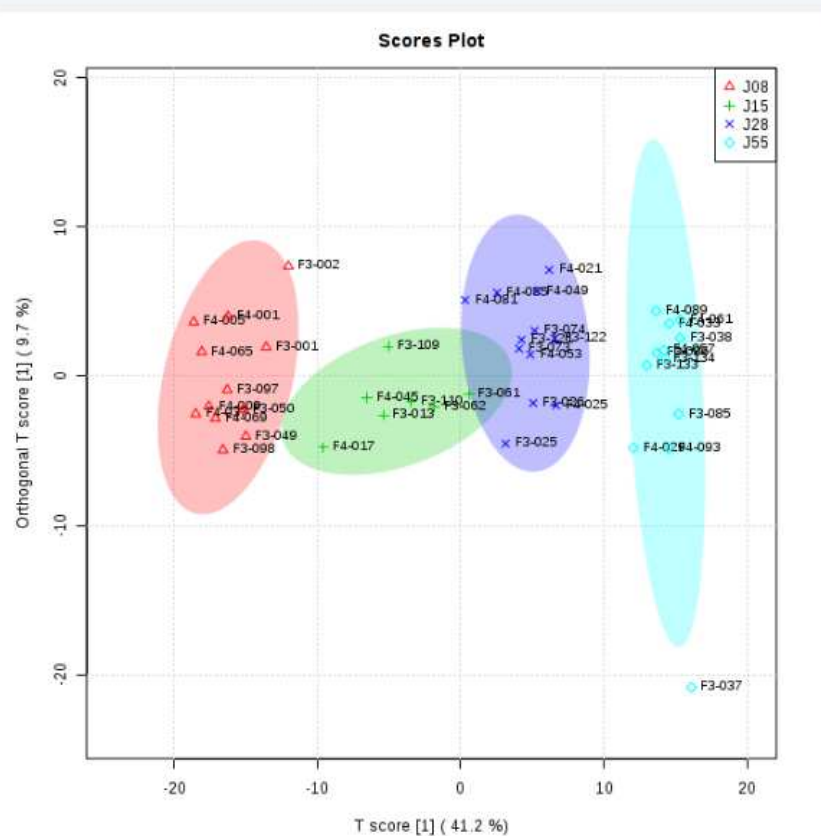
Set permutation numbers:

1000

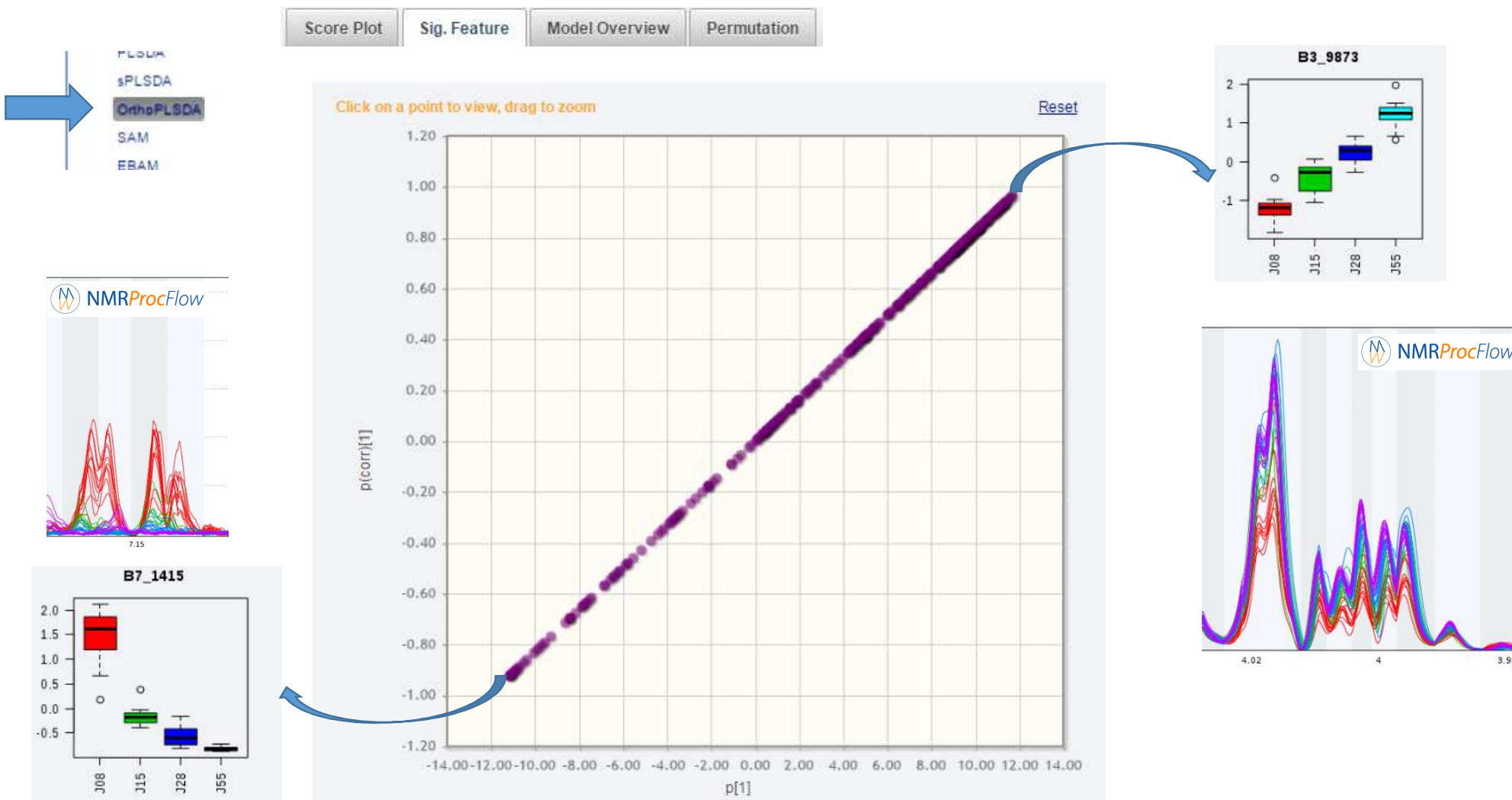
Submit

Processing ....

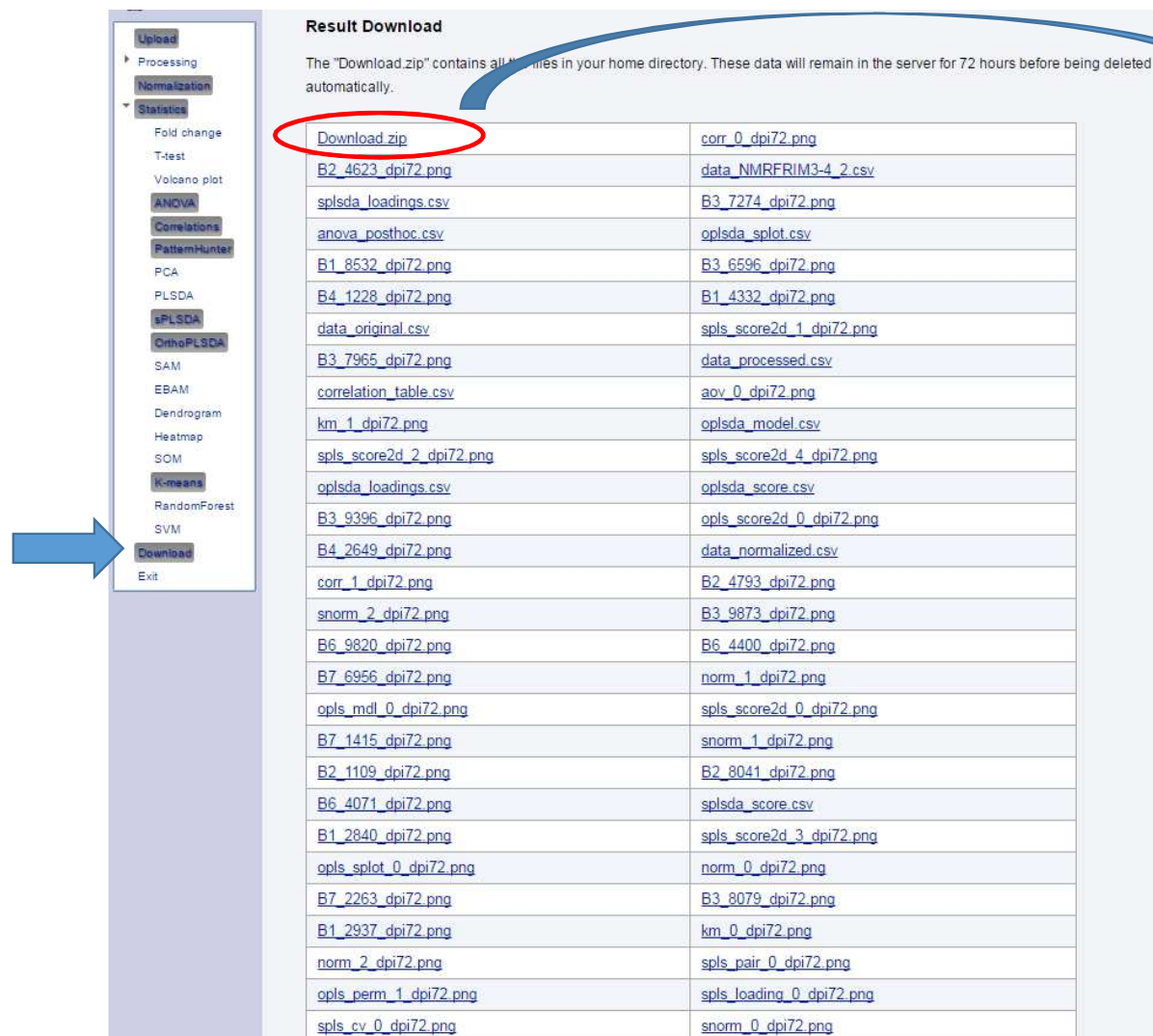
This may take a while to complete, please wait...



## A simple session with MetaboAnalyst 3.0



## A simple session with MetaboAnalyst 3.0



**Result Download**

The "Download.zip" contains all files in your home directory. These data will remain in the server for 72 hours before being deleted automatically.

<a href="#">Download.zip</a>	<a href="#">corr_0_dpi72.png</a>
<a href="#">B2_4623_dpi72.png</a>	<a href="#">data_NMRFRIM3-4_2.csv</a>
<a href="#">splstda_loadings.csv</a>	<a href="#">B3_7274_dpi72.png</a>
<a href="#">anova_posthoc.csv</a>	<a href="#">oplsda_splot.csv</a>
<a href="#">B1_8532_dpi72.png</a>	<a href="#">B3_6596_dpi72.png</a>
<a href="#">B4_1228_dpi72.png</a>	<a href="#">B1_4332_dpi72.png</a>
<a href="#">data_original.csv</a>	<a href="#">splstda_score2d_1_dpi72.png</a>
<a href="#">B3_7965_dpi72.png</a>	<a href="#">data_processed.csv</a>
<a href="#">correlation_table.csv</a>	<a href="#">aov_0_dpi72.png</a>
<a href="#">km_1_dpi72.png</a>	<a href="#">oplsda_model.csv</a>
<a href="#">splstda_score2d_2_dpi72.png</a>	<a href="#">splstda_score2d_4_dpi72.png</a>
<a href="#">oplsda_loadings.csv</a>	<a href="#">oplsda_score.csv</a>
<a href="#">B3_9396_dpi72.png</a>	<a href="#">opls_score2d_0_dpi72.png</a>
<a href="#">B4_2649_dpi72.png</a>	<a href="#">data_normalized.csv</a>
<a href="#">corr_1_dpi72.png</a>	<a href="#">B2_4793_dpi72.png</a>
<a href="#">snorm_2_dpi72.png</a>	<a href="#">B3_9873_dpi72.png</a>
<a href="#">B6_9820_dpi72.png</a>	<a href="#">B6_4400_dpi72.png</a>
<a href="#">B7_6956_dpi72.png</a>	<a href="#">norm_1_dpi72.png</a>
<a href="#">opls_md1_0_dpi72.png</a>	<a href="#">splstda_score2d_0_dpi72.png</a>
<a href="#">B7_1415_dpi72.png</a>	<a href="#">snorm_1_dpi72.png</a>
<a href="#">B2_1109_dpi72.png</a>	<a href="#">B2_8041_dpi72.png</a>
<a href="#">B6_4071_dpi72.png</a>	<a href="#">splstda_score.csv</a>
<a href="#">B1_2840_dpi72.png</a>	<a href="#">splstda_score2d_3_dpi72.png</a>
<a href="#">opls_splot_0_dpi72.png</a>	<a href="#">norm_0_dpi72.png</a>
<a href="#">B7_2263_dpi72.png</a>	<a href="#">B3_8079_dpi72.png</a>
<a href="#">B1_2937_dpi72.png</a>	<a href="#">km_0_dpi72.png</a>
<a href="#">norm_2_dpi72.png</a>	<a href="#">splstda_pair_0_dpi72.png</a>
<a href="#">opls_perm_1_dpi72.png</a>	<a href="#">splstda_loading_0_dpi72.png</a>
<a href="#">splstda_cv_0_dpi72.png</a>	<a href="#">snorm_0_dpi72.png</a>

anova\_posthoc.csv  
aov\_0\_dpi72.png  
B1\_2937\_dpi72.png  
B1\_8532\_dpi72.png  
B2\_4623\_dpi72.png  
B2\_8041\_dpi72.png  
B3\_7274\_dpi72.png  
B3\_8079\_dpi72.png  
B3\_9873\_dpi72.png  
B4\_2649\_dpi72.png  
B6\_4400\_dpi72.png  
B7\_1415\_dpi72.png  
B7\_6956\_dpi72.png  
corr\_1\_dpi72.pdf  
correlation\_table.csv  
data\_normalized.csv  
data\_processed.csv  
data\_original.csv  
km\_1\_dpi72.png  
km\_1\_dpi72.png  
norm\_0\_dpi72.png  
norm\_2\_dpi72.png  
norm\_2\_dpi72.pdf  
opls\_md1\_0\_dpi72.png  
opls\_perm\_1\_dpi72.png  
opls\_score2d\_0\_dpi72.png  
opls\_splot\_0\_dpi72.png  
oplsda\_model.csv  
oplsda\_splot.csv  
snorm\_1\_dpi72.png  
snorm\_2\_dpi72.png  
snorm\_2\_dpi72.png  
splstda\_loading\_0\_dpi72.png  
splstda\_pair\_0\_dpi72.png  
splstda\_score2d\_0\_dpi72.png  
splstda\_score2d\_2\_dpi72.png  
splstda\_score2d\_4\_dpi72.png  
splstda\_loadings.csv

aov\_0\_dpi72.pdf  
B1\_2840\_dpi72.png  
B1\_4332\_dpi72.png  
B2\_1109\_dpi72.png  
B2\_4793\_dpi72.png  
B3\_6596\_dpi72.png  
B3\_7965\_dpi72.png  
B3\_9396\_dpi72.png  
B4\_1228\_dpi72.png  
B6\_4071\_dpi72.png  
B6\_9820\_dpi72.png  
B7\_2263\_dpi72.png  
corr\_0\_dpi72.png  
corr\_1\_dpi72.png  
data\_NMRFRIM3-4\_2.csv  
data\_original.csv  
km\_0\_dpi72.png  
km\_1\_dpi72.png  
norm\_1\_dpi72.png  
norm\_2\_dpi72.png  
opls\_md1\_0\_dpi72.png  
opls\_perm\_1\_dpi72.png  
opls\_score2d\_0\_dpi72.png  
oplsda\_loadings.csv  
oplsda\_score.csv  
snorm\_0\_dpi72.png  
snorm\_2\_dpi72.png  
splstda\_cv\_0\_dpi72.png  
splstda\_loading\_0\_dpi72.png  
splstda\_pair\_0\_dpi72.png  
splstda\_score2d\_1\_dpi72.png  
splstda\_score2d\_3\_dpi72.png  
splstda\_score2d\_4\_dpi72.png  
splstda\_score.csv





A simple session with MetaboAnalyst 3.0

**MetaboAnalyst 3.0**  
– a comprehensive tool suite for metabolomic data analysis

[Home](#)  
[Overview](#)  
[Data Formats](#)  
[FAQs](#)  
[Tutorials](#)  
[Troubleshooting](#)  
[Resources](#)  
[Update History](#)  
[User Stats](#)  
[About](#)

**Tutorial:**

The web interfaces of MetaboAnalyst are designed to be self-explanatory. Most steps are documented on top of the corresponding pages. In cases of limited space, mouse-over balloon helps are available. The following tutorials are meant to complement the aforementioned information by providing step-by-step instructions for several most common tasks. The analysis reports are the PDF report automatically generated by MetaboAnalyst following these steps.

Please note, due to the rapid evolution and frequent updates of MetaboAnalyst, many screenshot illustrations are outdated. Therefore, we ask users do not take those steps verbatim. Instead, users should focus on the the analysis steps and the workflow for metabolomics data analysis using the tool.

	Identification of significant features	Analysis report
	Two-group classification	Analysis report
	MS spectra processing and annotation	Analysis report
	Paired (two time-points) analysis	Analysis report
	Metabolomics data analysis I	* presented on Metabolomics Conference 2009
	Metabolomics data analysis II	* presented on Metabolomics Conference 2010
	Metabolomics data analysis III	* presented on Metabolomics Conference 2011
	Metabolomics data analysis IV	* presented on Metabolomics Conference 2012
	Nature Protocols on MetaboAnalyst	Detailed explanations of major functions of MetaboAnalyst
	Current Protocols In Bioinformatics	A comprehensive step-by-step tutorial (48 pages & 51 figures)
	Raw Spectra Processing using R and XCMS	Step-by-step tutorial to processing LC-MS spectra for MetaboAnalyst

The better now it's to read the plenty online tutorials so that you could find your happiness !