NMRProcFlow

MetaboAnalyst 3.0
– a comprehensive tool suite for metabolomic data analysis

A simple session with MetaboAnalyst 3.0 (Nov. 2016)

Perform statistical analysis using MetaboAnalyst on exported data from NMRProcFlow

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INRA UMR 1332 Biologie du Fruit et Pathogènes

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Data Export

NMRProcFlow

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_6955	B7_6635	B7_4512	B7_4362	B7_4224	B7_4090	B7_3957	B7_3834	B7
F3-001	Control	J08	0.11928791	0.00581534	0.16150283	0.047086	0.09814824	0.09813412	0.01898936	0.03941068	0.04948976	0.02022299	0.00373654	0.02378087	0
F3-049	Control	J08	0.10384242	0.00835102	0.13589457	0.06153699	0.14618564	0.14036055	0.01539754	0.01692683	0.01200164	0.01717897	0.01085015	0.02315004	0
F3-097	Control	J08	0.09651629	0.00523615	0.17433857	0.06213409	0.16545419	0.18503065	0.02161687	0.0214187	0.02813971	0.02358135	0.01270131	0.02834738	0
F3 002	Shadow	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
F3-050	Shadow	J08	0.12598911	0.01304445	0.13824284	0.05809637	0.14485492	0.13533937	0.03232633	0.01034411	0.01846426	0.02983426	0.02225713	0.03401898	
F3-098	Shadow	J08	0.12360064	0.00724083	0.12727933	0.05951439	0.17228324	0.16153312	0.04384093	0.01533951	0.01755694	0.03644395	0.01806933	0.0301551	0
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
F3-061	Control	J15	0.05667186	0.00552217	0.08759005	0.04733081	0.03781117	0.03933464	0.02078347	0.05830485	0.07758045	0.0348291	0.01933022	0.03107577	0
F3-109	Control	J15	0.07548592	0.0043453	0.08755526	0.04697576	0.05321745	0.05536447	0.00768144	0.0600623	0.08110839	0.03416974	0.01394663	0.03504505	0
F3-062	Shadow	J15	0.05708147	0.00229657	0.07625981	0.04703255	0.03478351	0.02437456	0.01564896	0.04840928	0.0614291	0.02940266	0.01571519	0.02557809	0
F3-110	Shadow	J15	0.08843008	0.00366854	0.11023306	0.04240016	0.04629357	0.0565123	0.02686256	0.03765864	0.046656	0.02001858	0.01410188	0.02813436	0
F3-025	Control	J28	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
F3-073	Control	J28	0.05267122	0.0042229	0.09108597	0.03208542	0.04221378	0.02215247	0.02931834	0.07019428	0.0875616	0.04330502	0.02846465	0.04251691	0
F3-121	Control	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
F3-026	Shadow	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	
F3-074	Shadow	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	
F3 122	Shadow	J28	0.05738645	0.00203373	0.06196753	0.04248531	0.02371078	0.01953007	0.03795215	0.08552814	0.10944816	0.04647477	0.03542677	0.04118655	0
F3-037	Control	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
F3-085	Control	J55	0.06712416	0.06835656	0.10970451	0.11024554	0.01595192	0.00922174	0.028818	0.07459614	0.07824352	0.02872809	0.04676672	0.03166962	0
F3-133	Control	J55	0.04319144	0.08858712	0.121372	0.13439019	0.00701526	0.01108497	0.02752508	0.09864951	0.11831952	0.04516909	0.05693713	0.04737119	0
F3-038	Shadow	J55	0.07895642	0.12345603	0.1278891	0.1784346	0.00541509	0.0076085	0.03272434	0.10715168	0.12007041	0.04038197	0.05594181	0.04416299	0
F3-086	Shadow	J55	0.07690517	0.09031835	0.12895596	0.14985144	0.01430116	0.00886306	0.01626272	0.06070653	0.07374108	0.02860104	0.05225686	0.02533339	0
F3-134	Shadow	J55	0.05143253	0.1055738	0.12450084	0.14763796	0.01646724	0.00440021	0.03385417	0.11258537	0.12189743	0.04185418	0.04906765	0.04550948	0
F4-001	Control	J08	0.1230095	0.0089157	0.16097331	0.05711878	0.14520576	0.16760372	0.03105041	0.03127852	0.03201556	0.02952918	0.02039009	0.0337445	

2 factors

...

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

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Data Preparation

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.(
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.(
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.(
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.(
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.(
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.(
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.(
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.(
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.(
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.(
13	F3-025	J28	0.04971968	0.00192048	0.07801866	0.02777739	0.05304738	0.02581476	0.00771899	0.05555394	0.06138559	0.03070073	0.01540366	0.02825725	0.03624349	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.(
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.(
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.(
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.(
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.(
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.(
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.(
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.(
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.(
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.(
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.(
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	
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.(
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.(
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.(

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

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A simple session with MetaboAnalyst 3.0

http://www.metaboanalyst.ca

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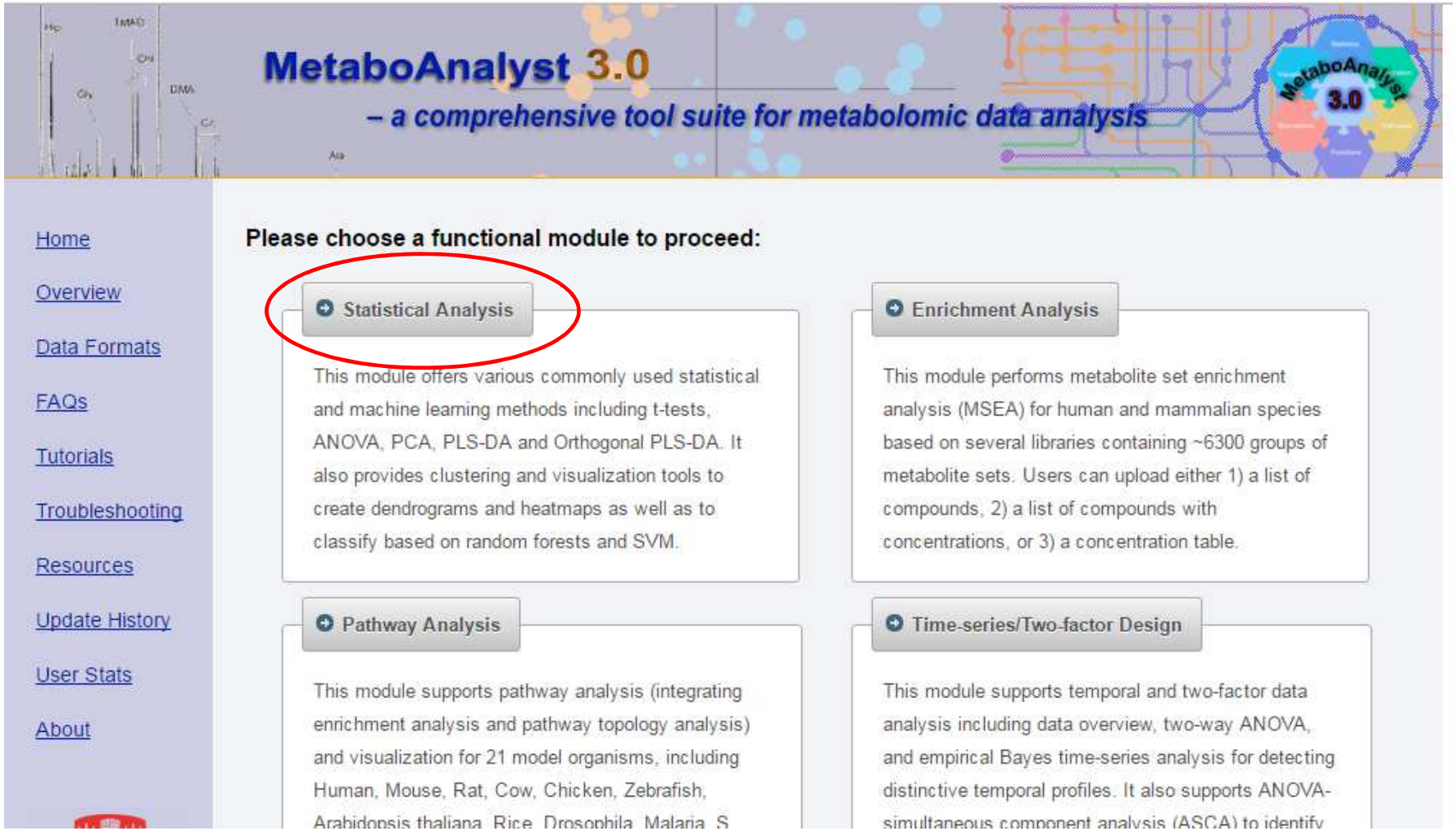
A simple session with MetaboAnalyst 3.0



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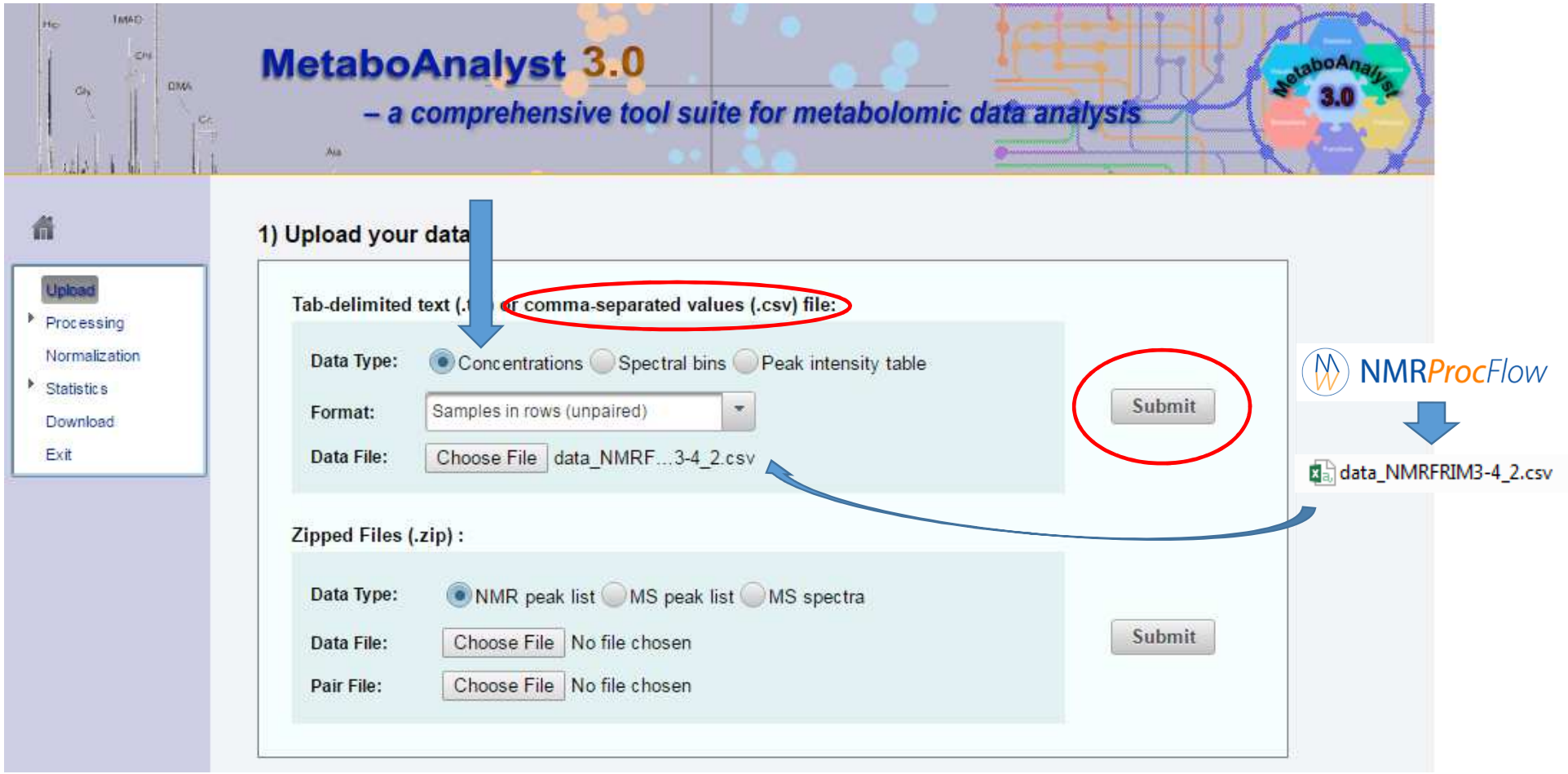
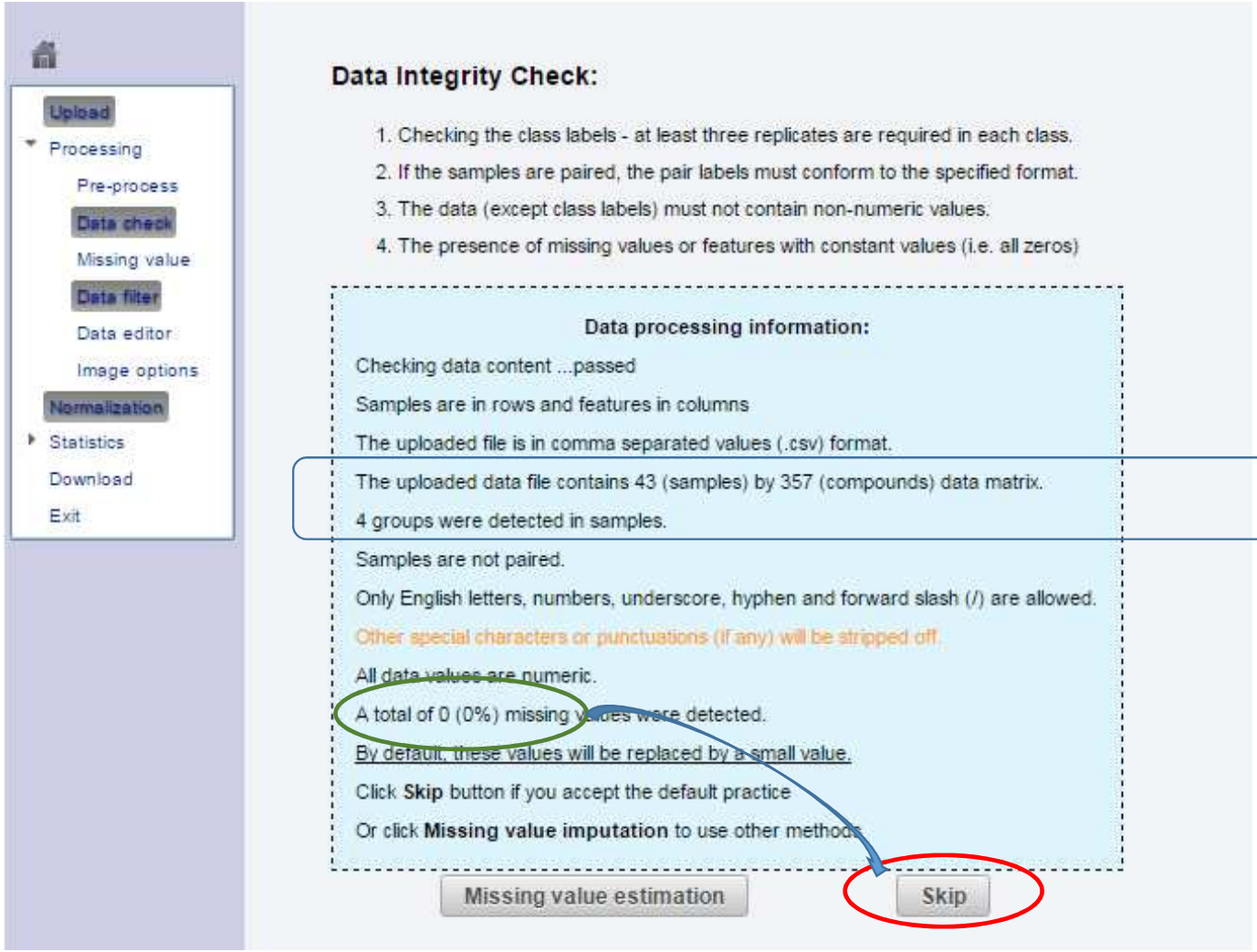
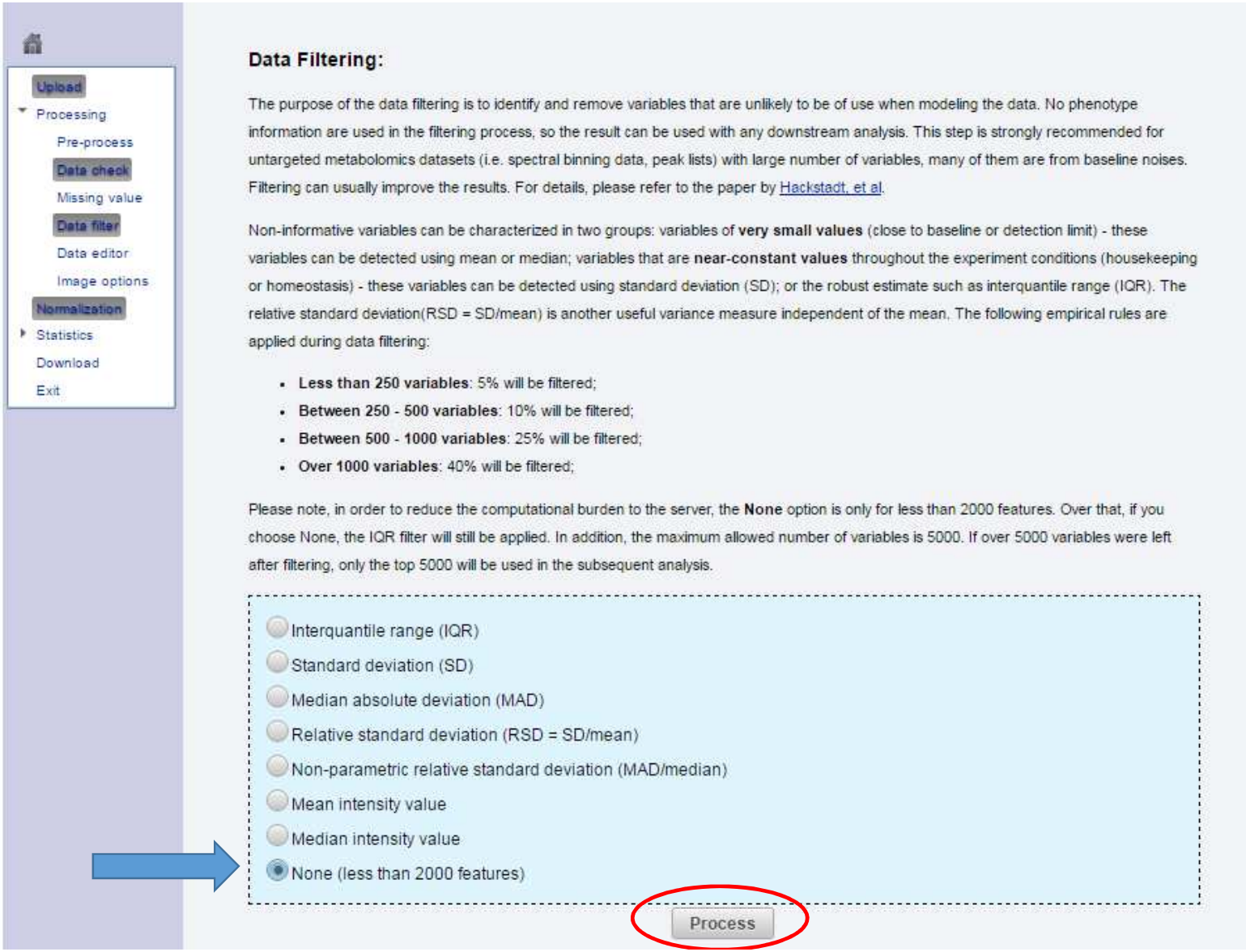


A simple session with MetaboAnalyst 3.0



OK



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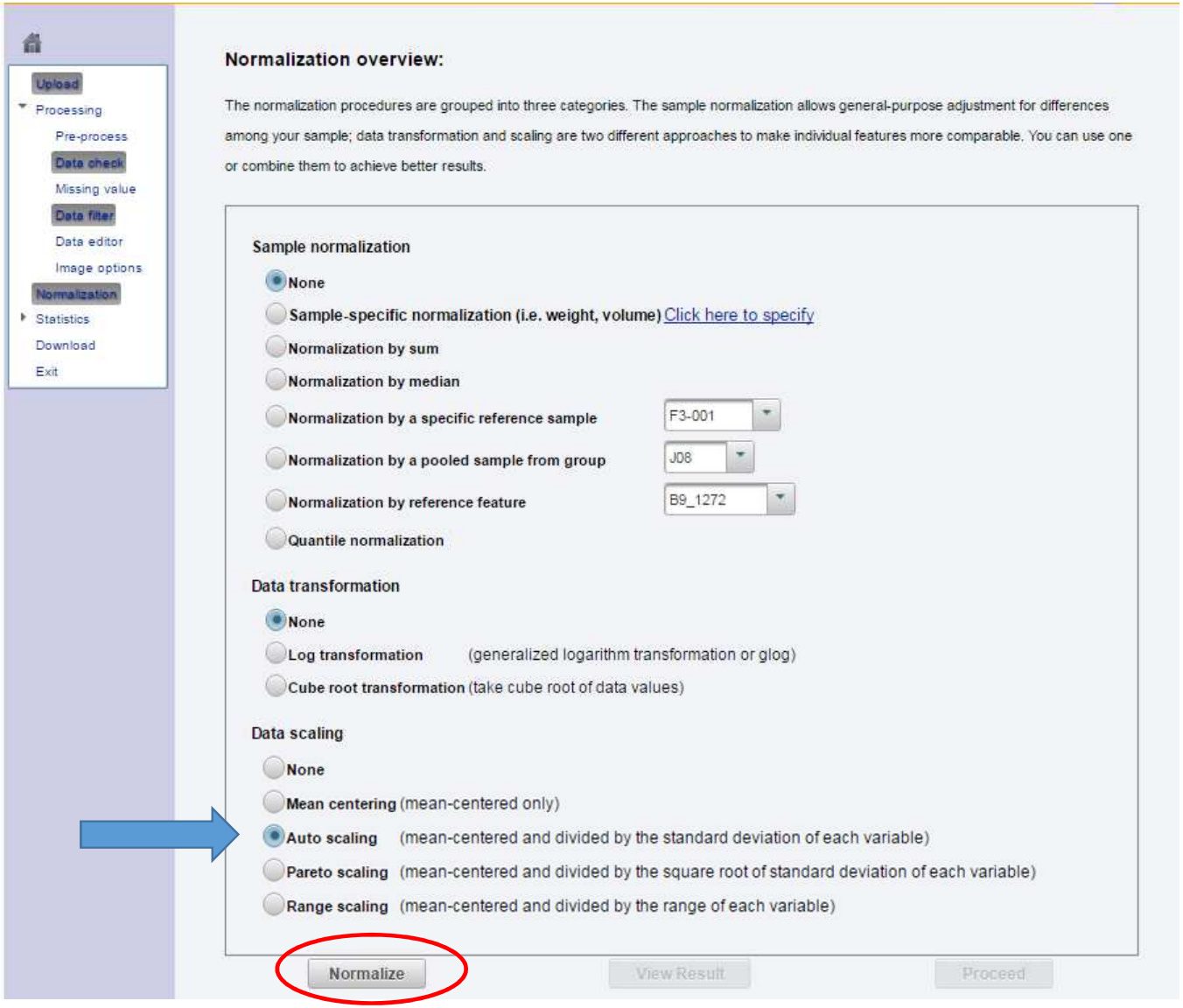

NMRProcFlow

Normalization Method:

Constant Sum Normalization

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

SNR threshold:

3

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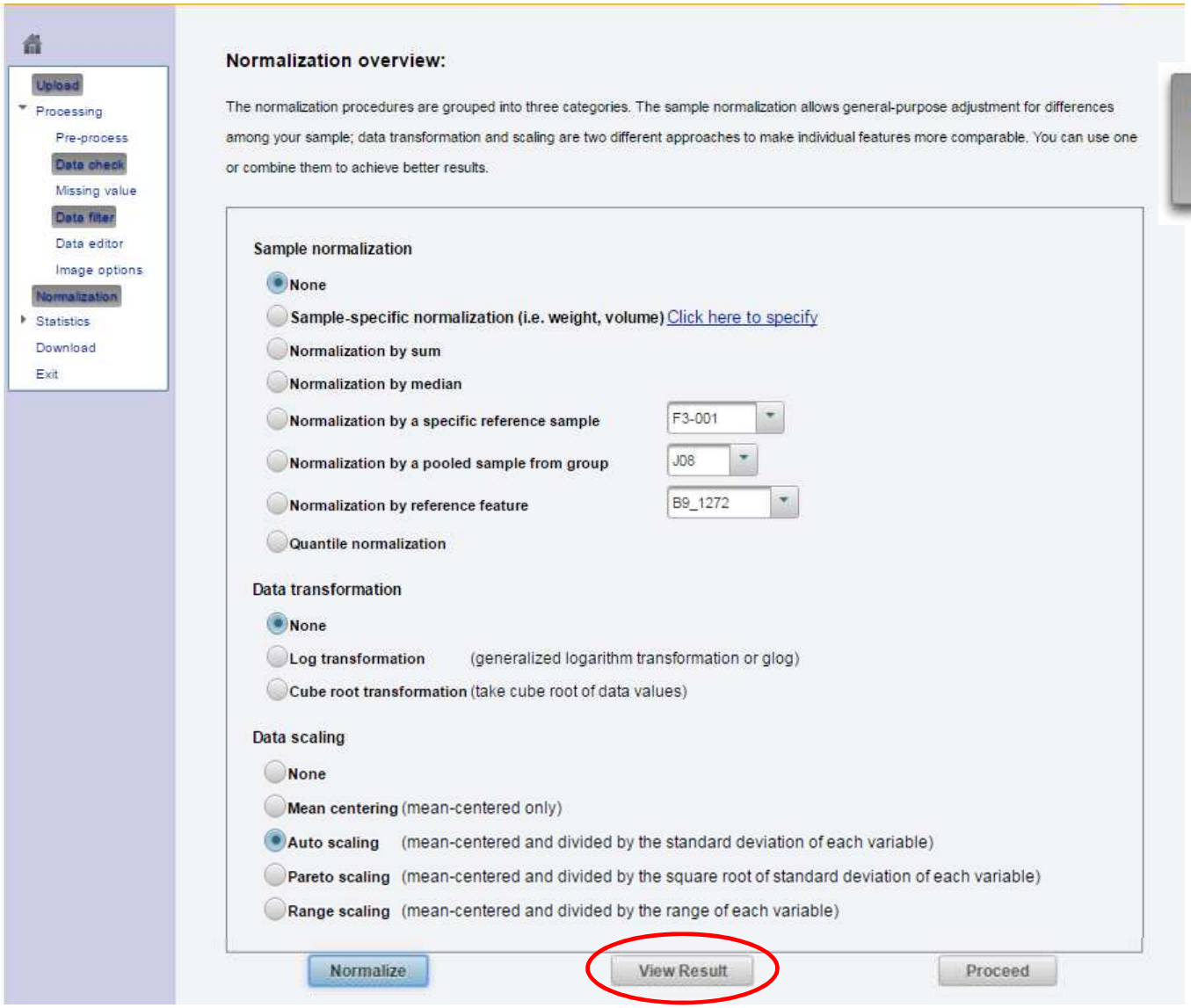

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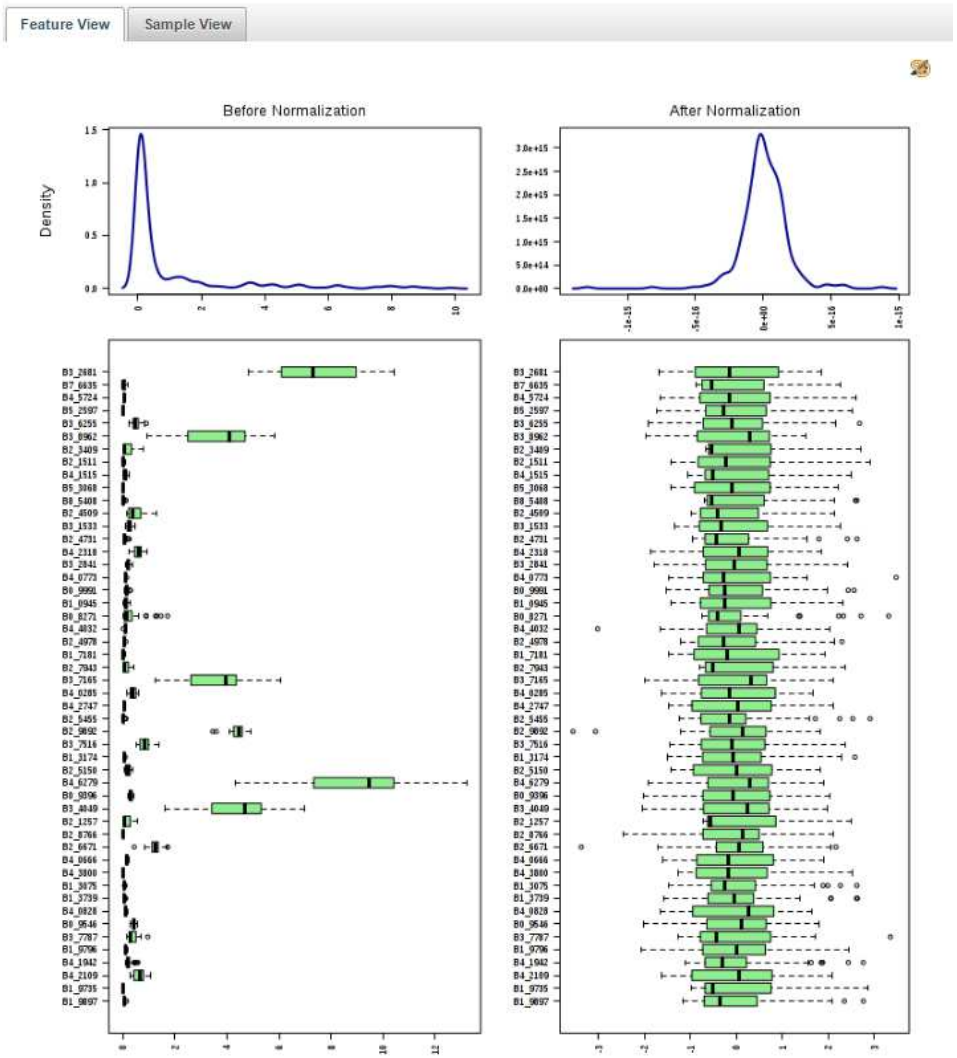

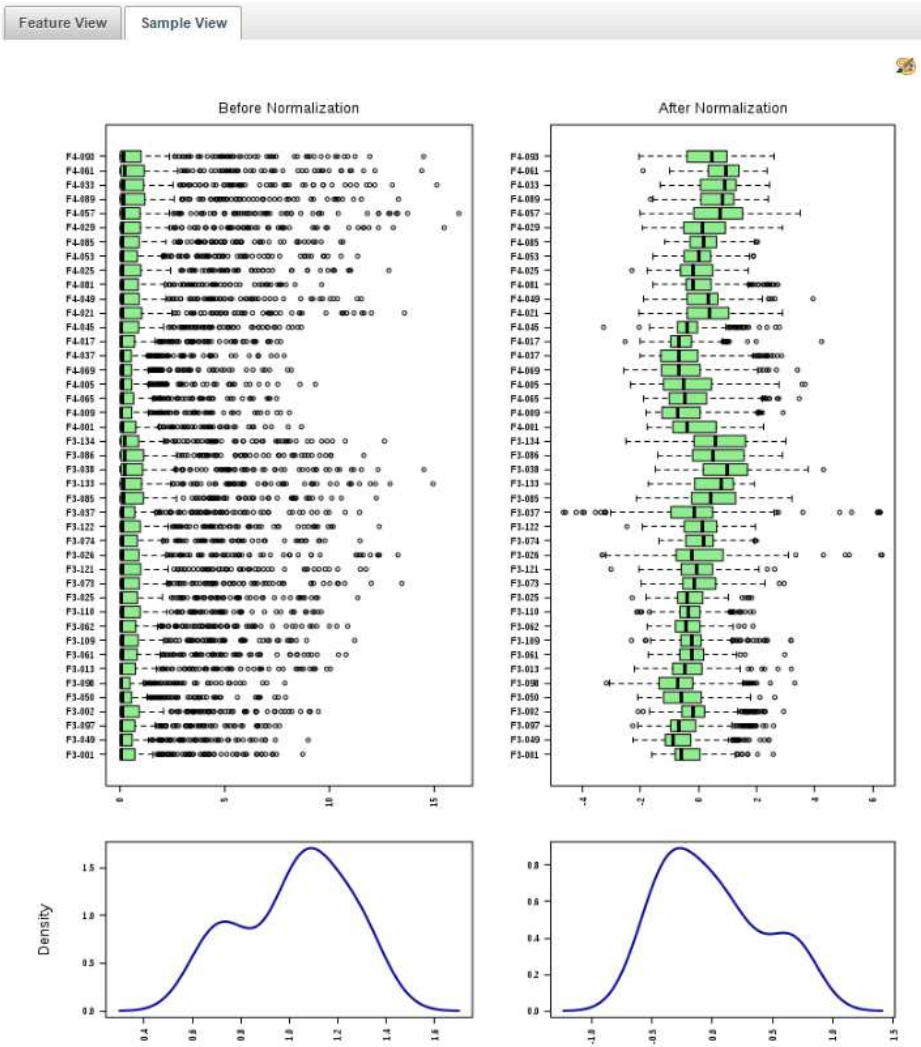

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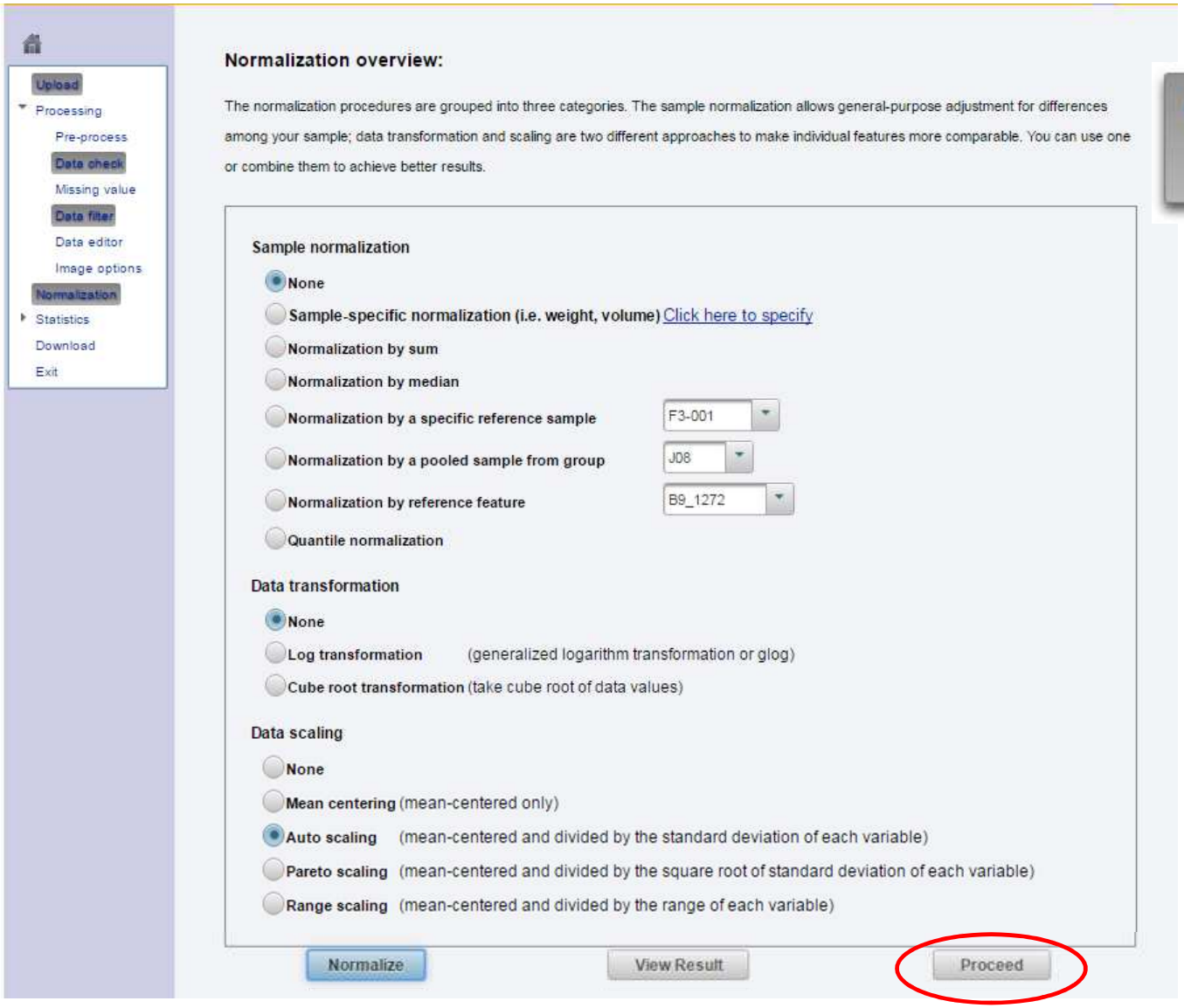

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– a comprehensive tool suite for metabolomic data analysis

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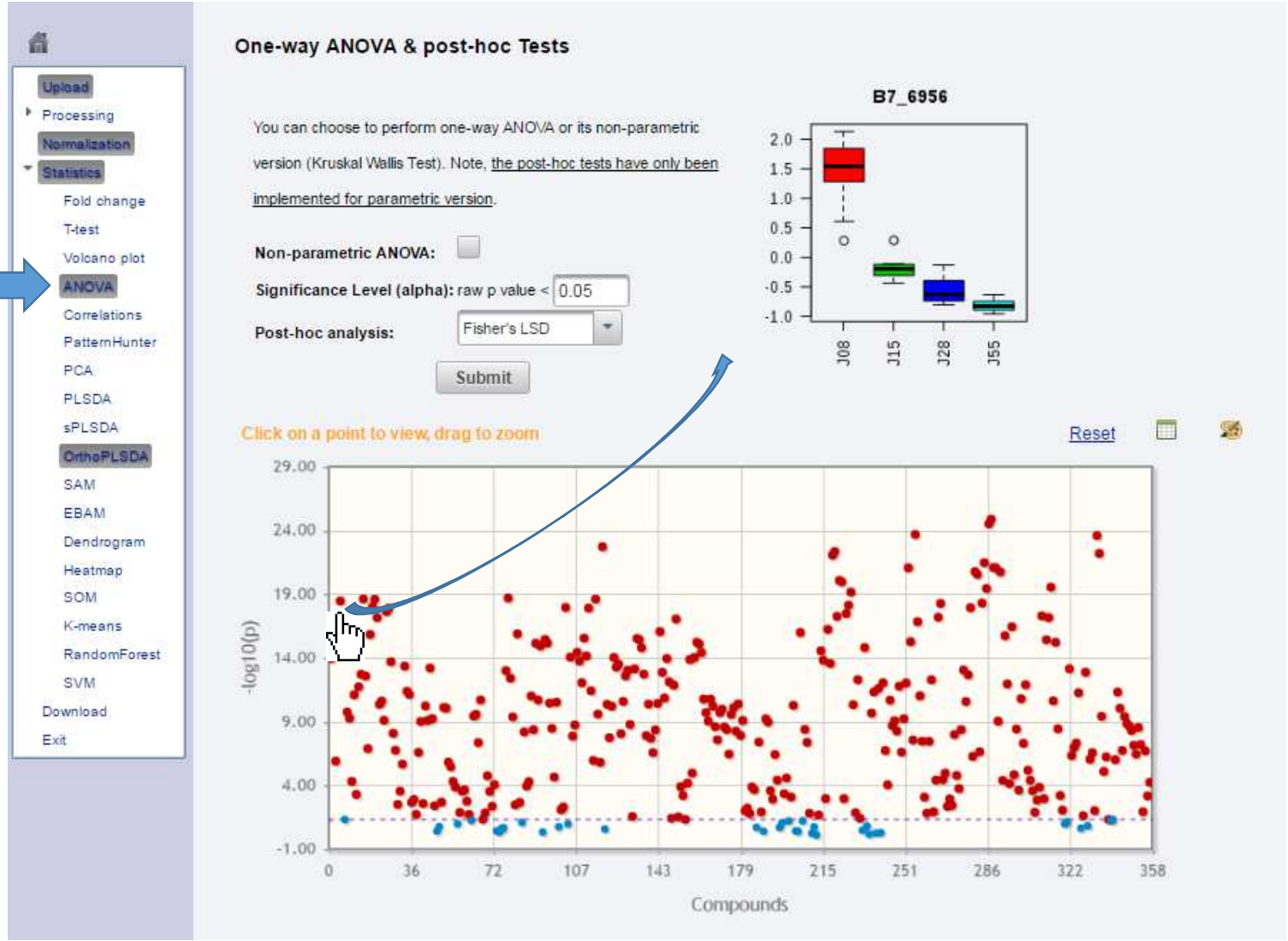

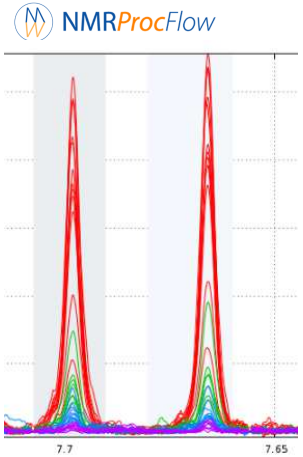

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MetaboAnalyst 3.0
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Upload
Processing
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Fold change
T-test
Volcano plot
ANOVA
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PatternHunter
PCA
PLSDA
sPLSDA
OrthoPLSDA
SAM
EBAM
Dendrogram
Heatmap
SOM
K-means
RandomForest
SVM
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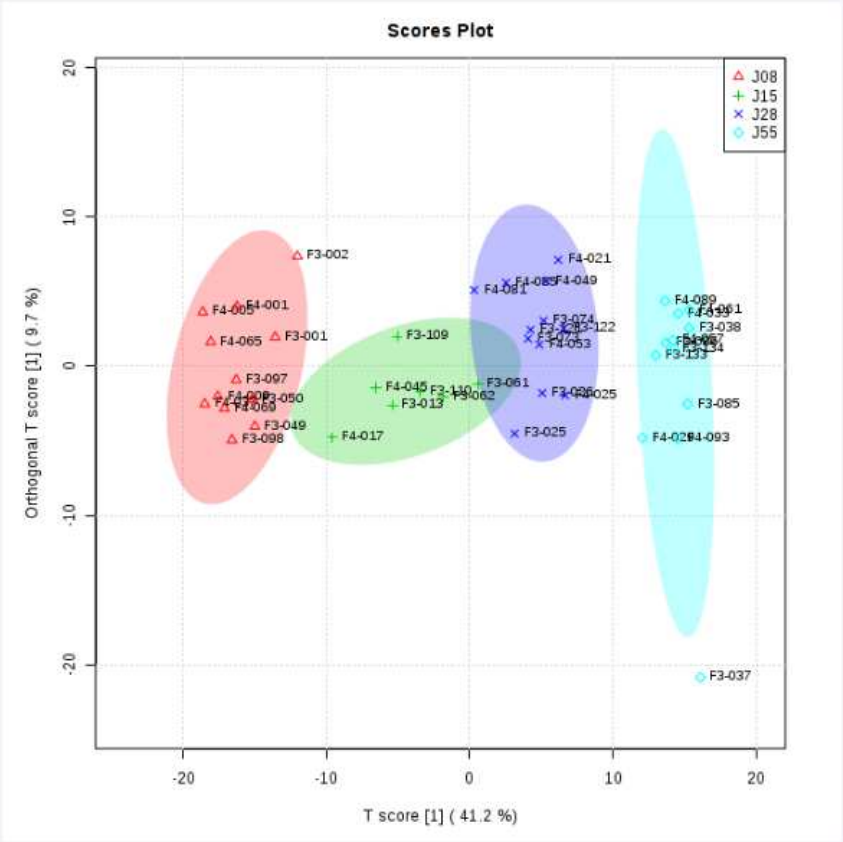
Orthogonal PLS-DA in MetaboAnalyst is based on PLS regression by converting the group labels into integers (Y) according to their numerical or alphabetic orders. The scores, loadings, R2 and Q2 are computed from the regression model based on both X and Y.
Make sure the group labels are consistent when you compare models on the same data (X).

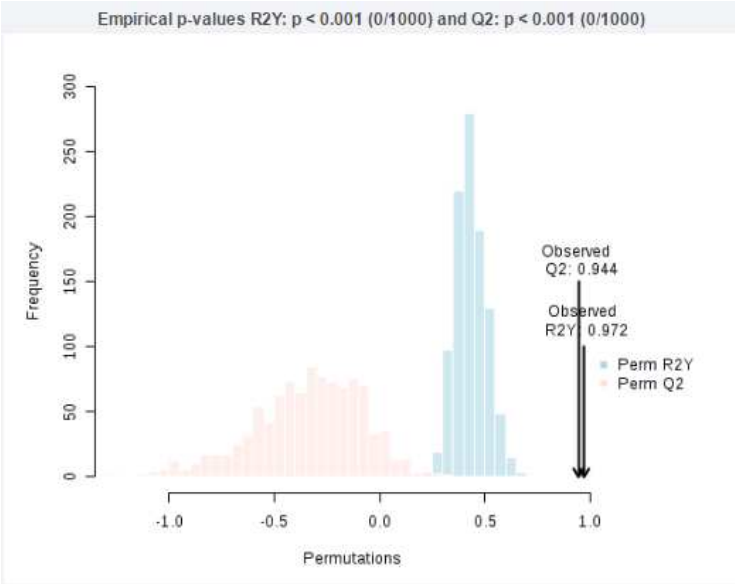
Score Plot | Sig. Feature | Model Overview | Permutation

Display 95% confidence region: ☑
Display sample names: ☑ Update
Use grey-scale colors: ☐

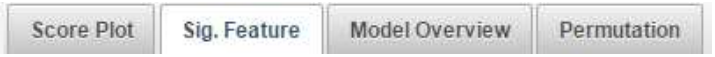


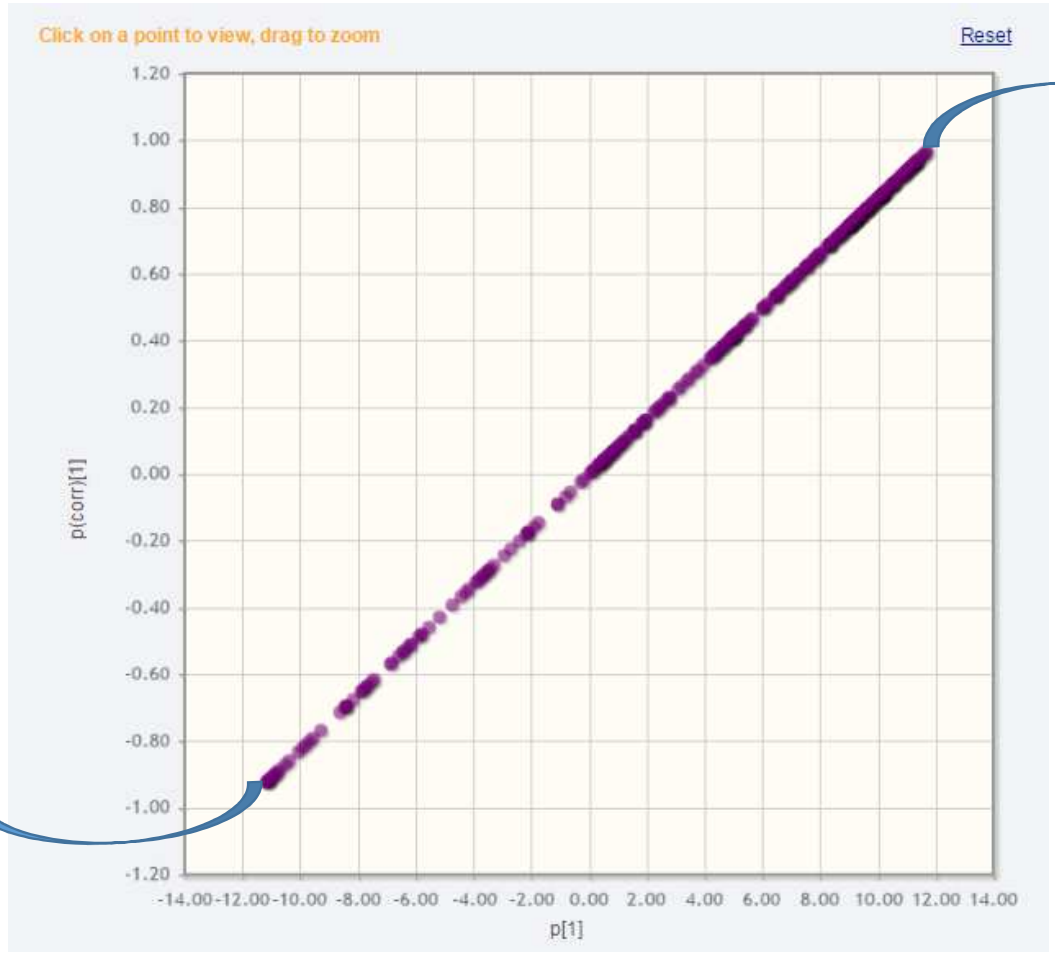
Set permutation numbers: 1000 Submit

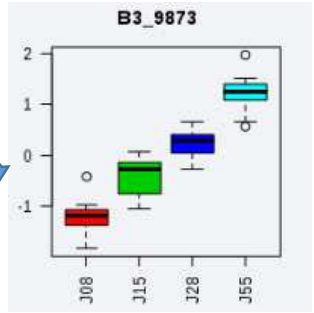
Processing ....
This may take a while to complete, please wait....

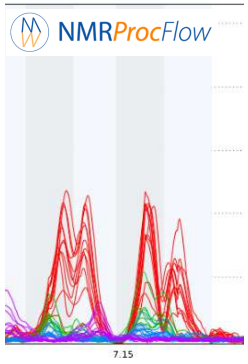


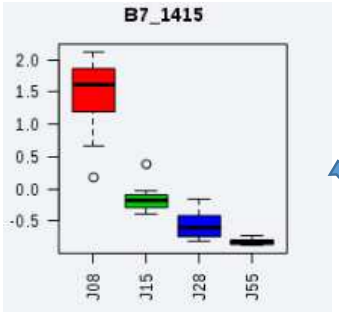
A simple session with MetaboAnalyst 3.0

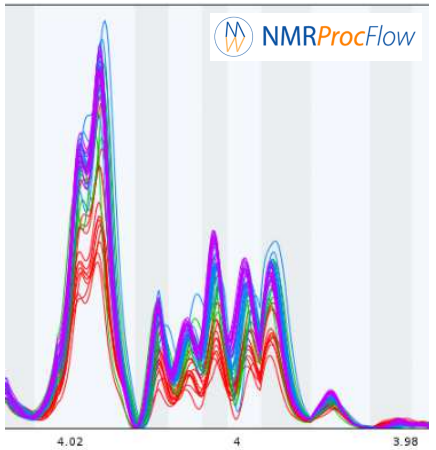












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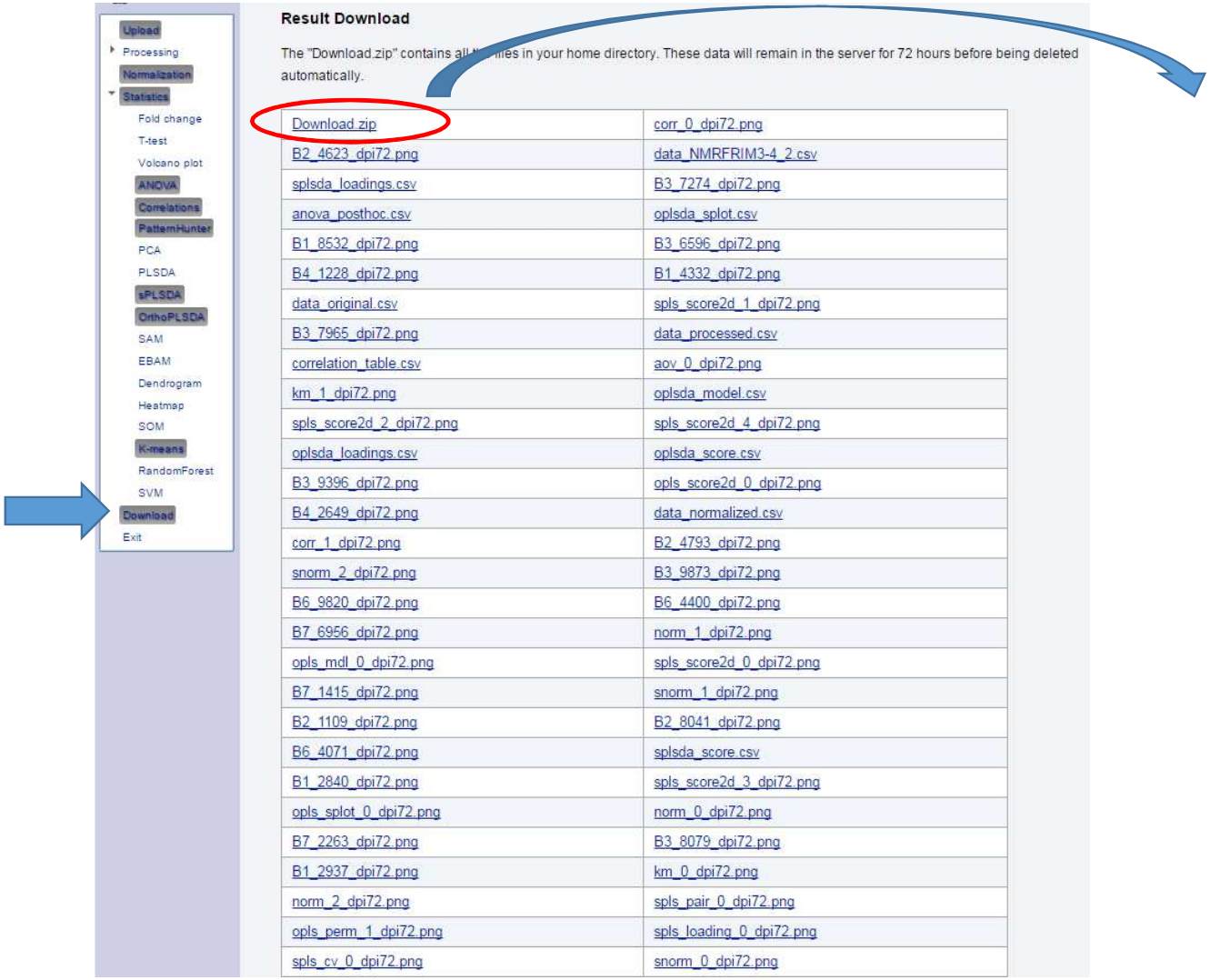

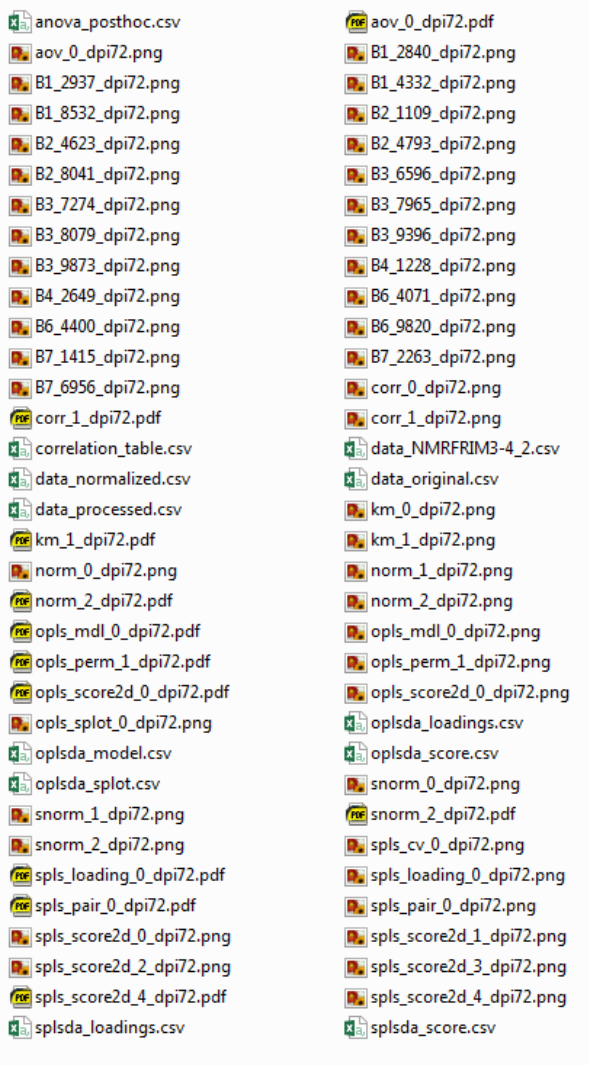

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The better now it's to read the plenty online tutorials so that you could find your happiness !

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