Statistical analysis with Metaboanalyst

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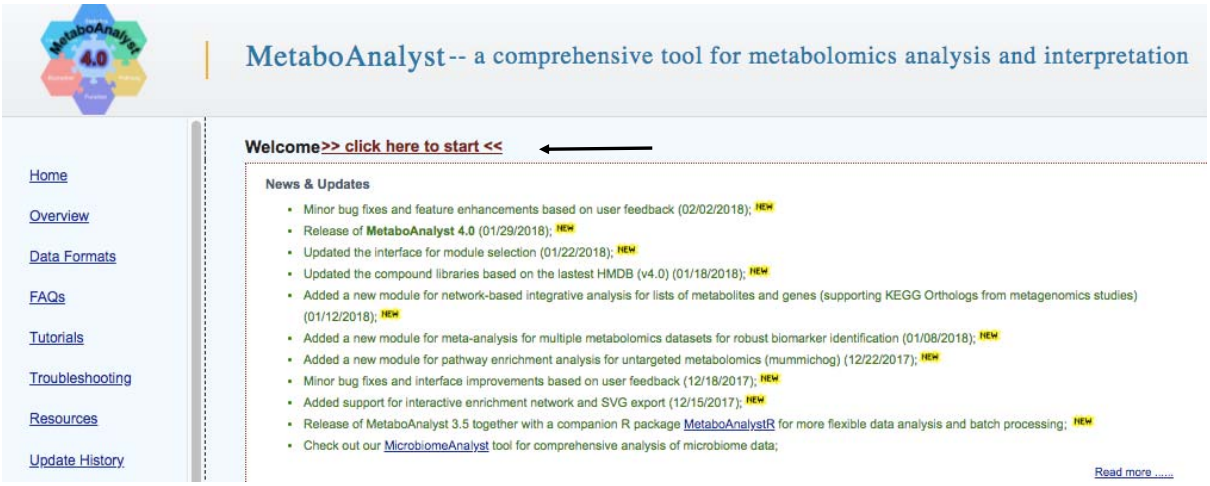
Go to www.metaboanalyst.ca



Jeff Xia

Othman Soufan
Jordan

Iurie Caraus
Moldova

Charles Viau
Canada

Guangyan Zhou
China

Jasmine Chong
Canada

Orcun Hacariz
Turkey

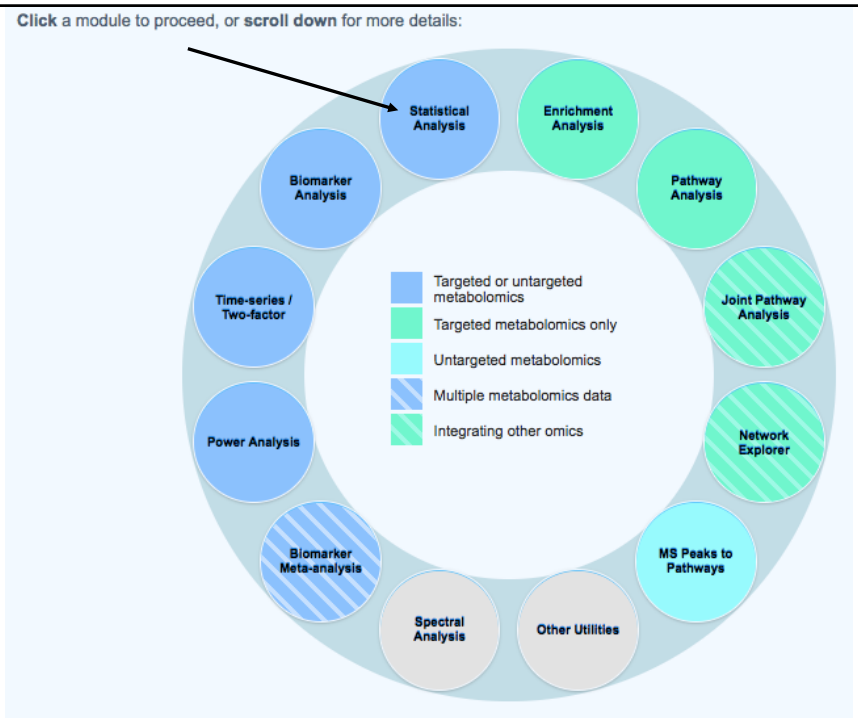
Honghao Zhao
China

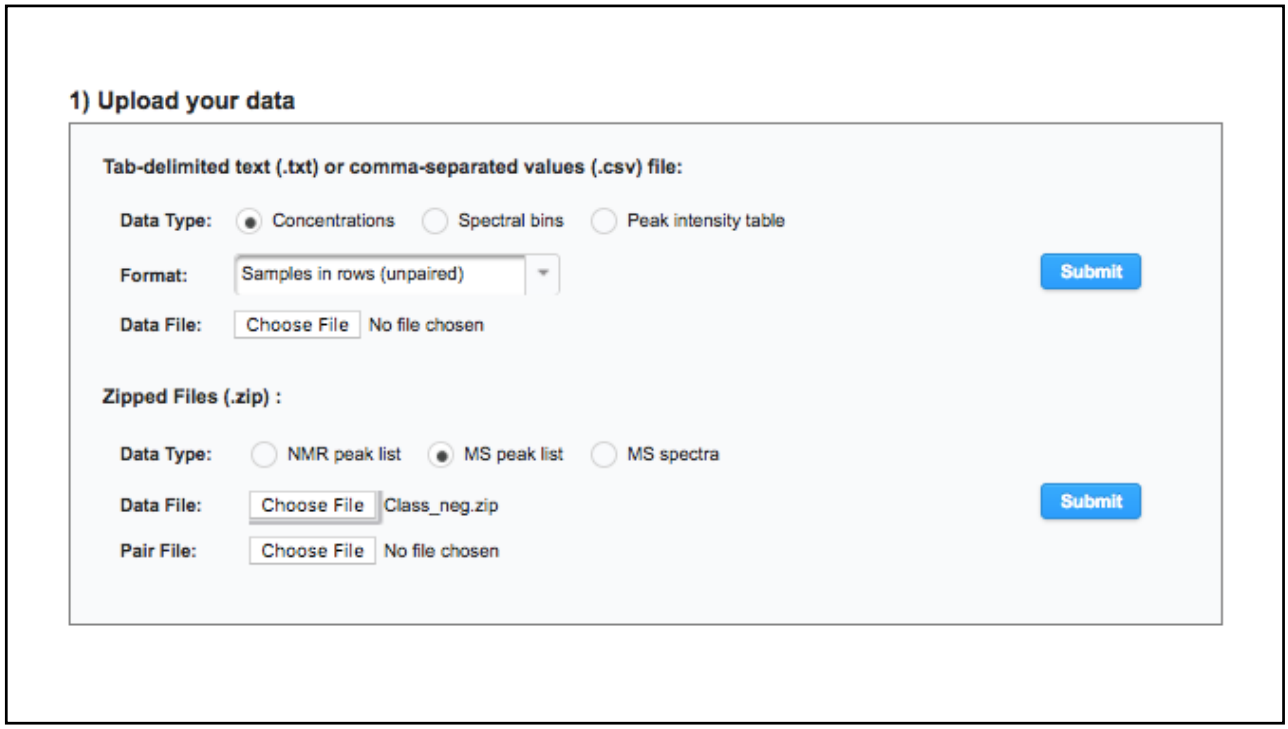
Achal Dhariwal
India

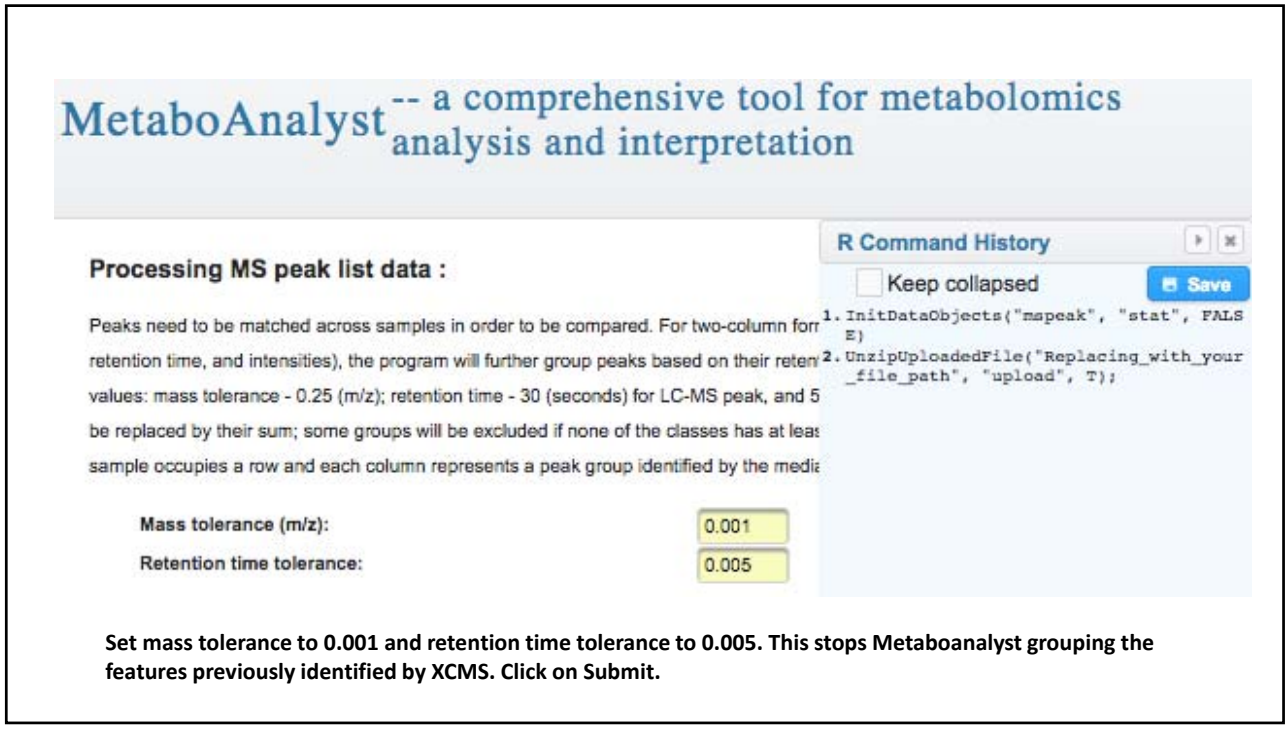
Yannan Fan
China

Deepak Tanwar
India

Maria Habib
Jordan







Set mass tolerance to 0.001 and retention time tolerance to 0.005. This stops Metaboanalyst grouping the features previously identified by XCMS. Click on Submit.

MS peak processing information

The uploaded files are peak lists and intensities data.

A total of 12 samples were found.

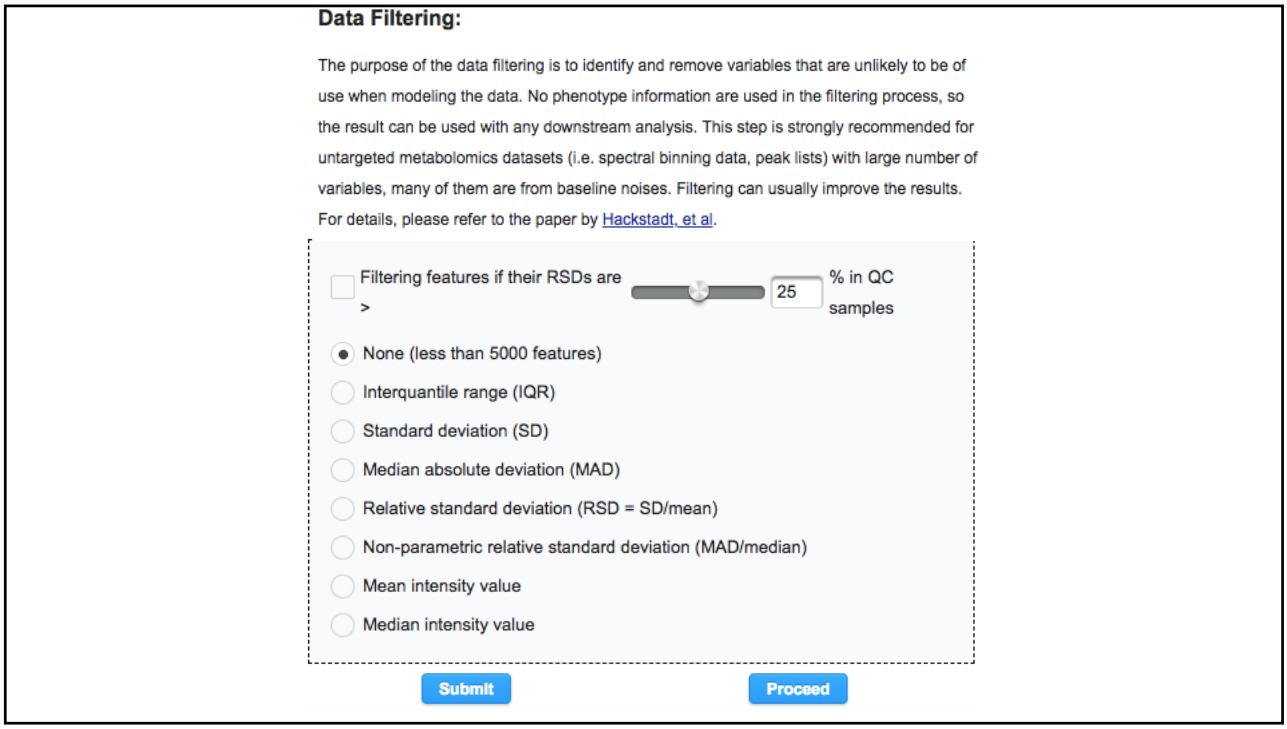
These samples contain a total of 39096 peaks,

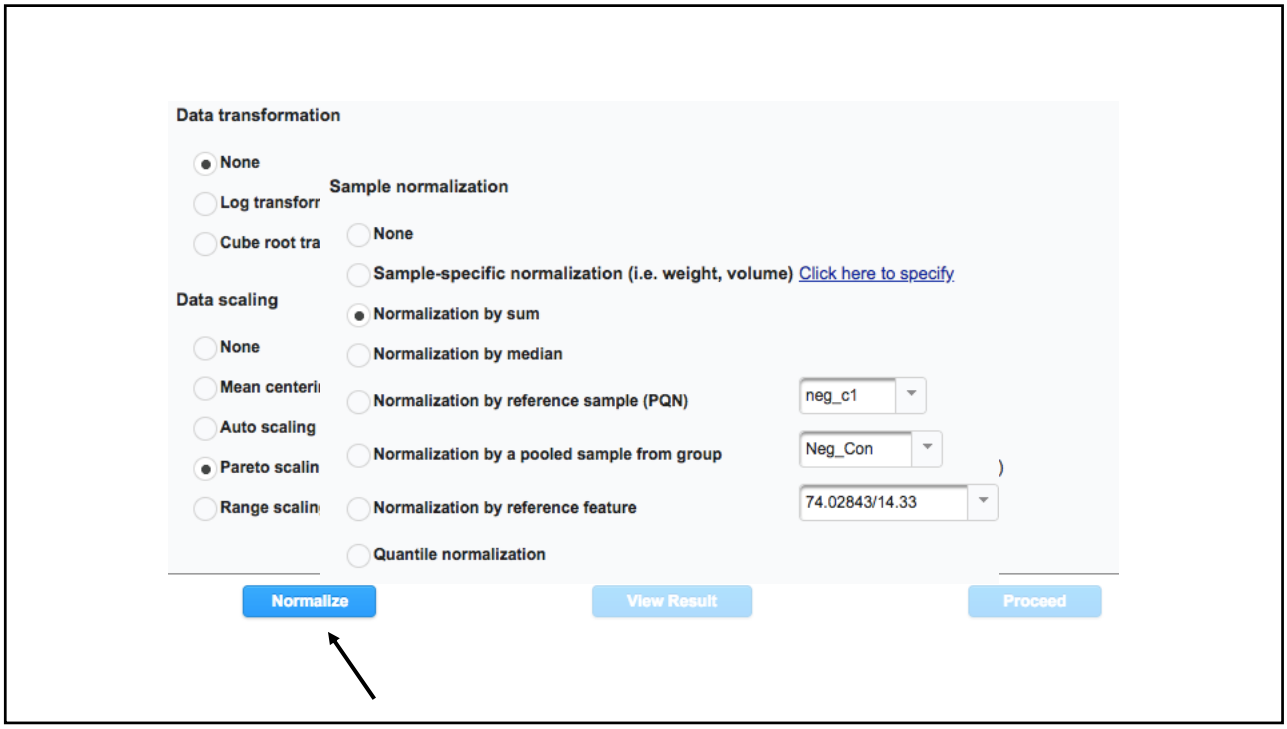
with an average of 3258 peaks per sample

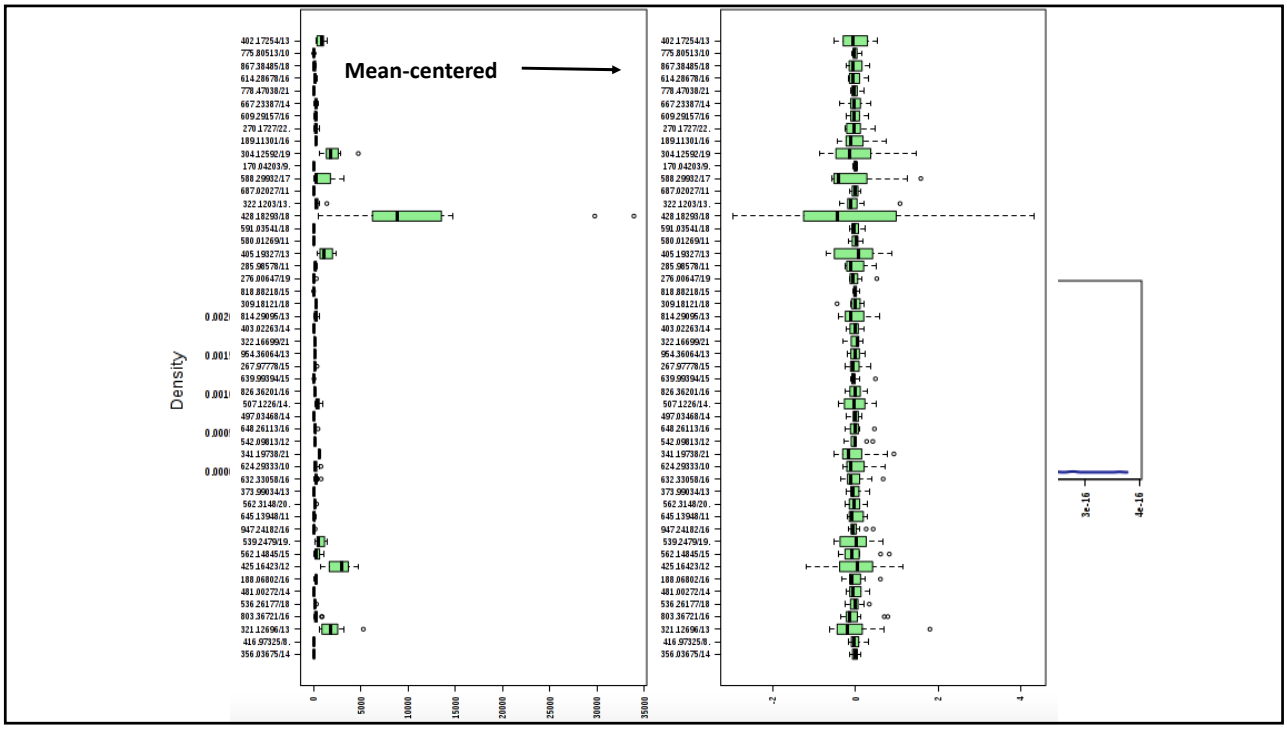
A total of 3258 peak groups were formed.

Peaks of the same group were summed if they are from one sample.

Peaks appearing in less than half of all samples in each group were ignored.


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.
Filtering features if their RSDs are >
25
% in QC samples
None (less than 5000 features)
Interquantile 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
Submit
Proceed


Data transformation
None
Log transforr
Cube root tra
Data scaling
None
Mean centeri
Auto scaling
Pareto scalin
Range scalin
Sample normalization
None
Sample-specific normalization (i.e. weight, volume) Click here to specify
Normalization by sum
Normalization by median
Normalization by reference sample (PQN)
neg_c1
Normalization by a pooled sample from group
Neg_Con
Normalization by reference feature
74.02843/14.33
Quantile normalization
Normalize
View Result
Proceed



Ready for Stats?

Univariate Analysis

Fold Change Analysis T-tests Volcano plot

One-way Analysis of Variance (ANOVA)

Correlation Analysis Pattern Searching

Chemometrics Analysis

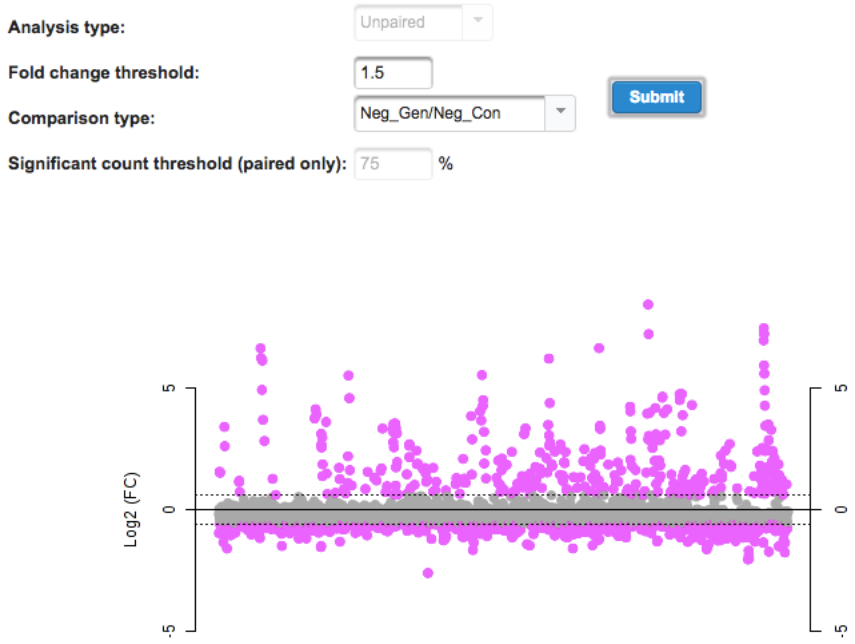
Principal Component Analysis (PCA)

Partial Least Squares - Discriminant Analysis (PLS-DA)

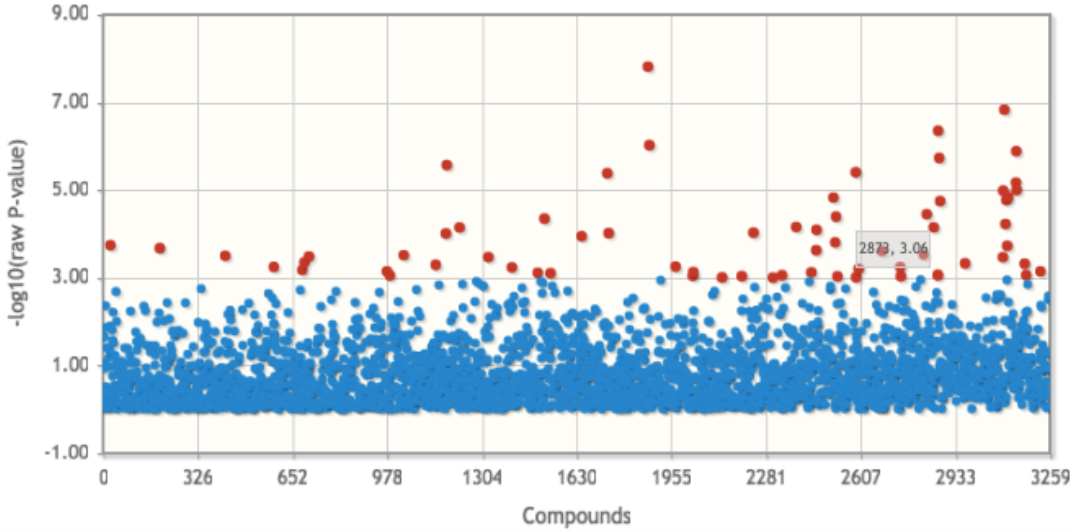
Sparse Partial Least Squares - Discriminant Analysis (sPLS-DA)

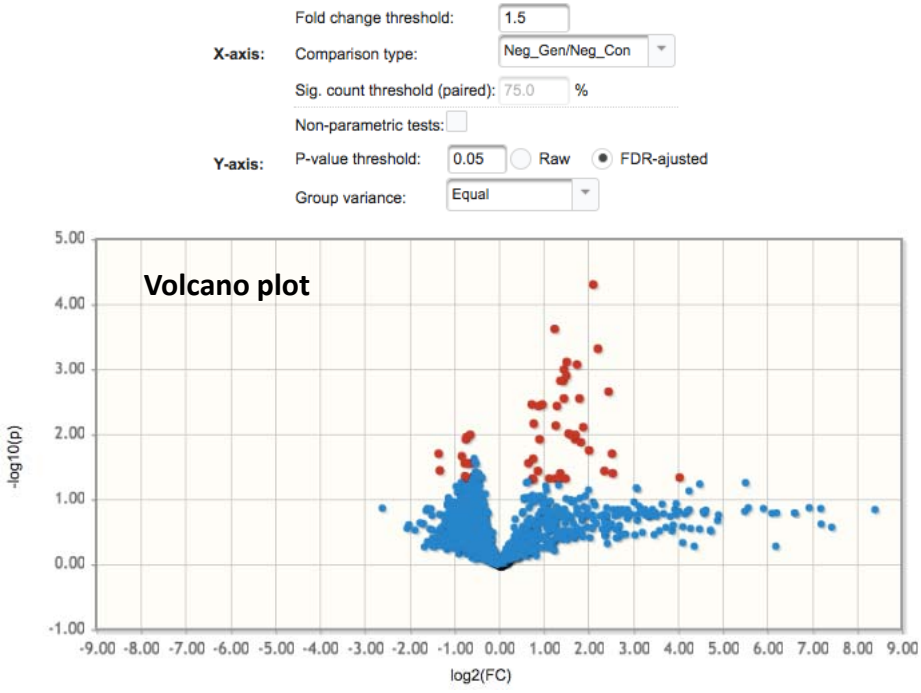
Orthogonal Partial Least Squares - Discriminant Analysis (orthoPLS-DA)

Univariate analysis

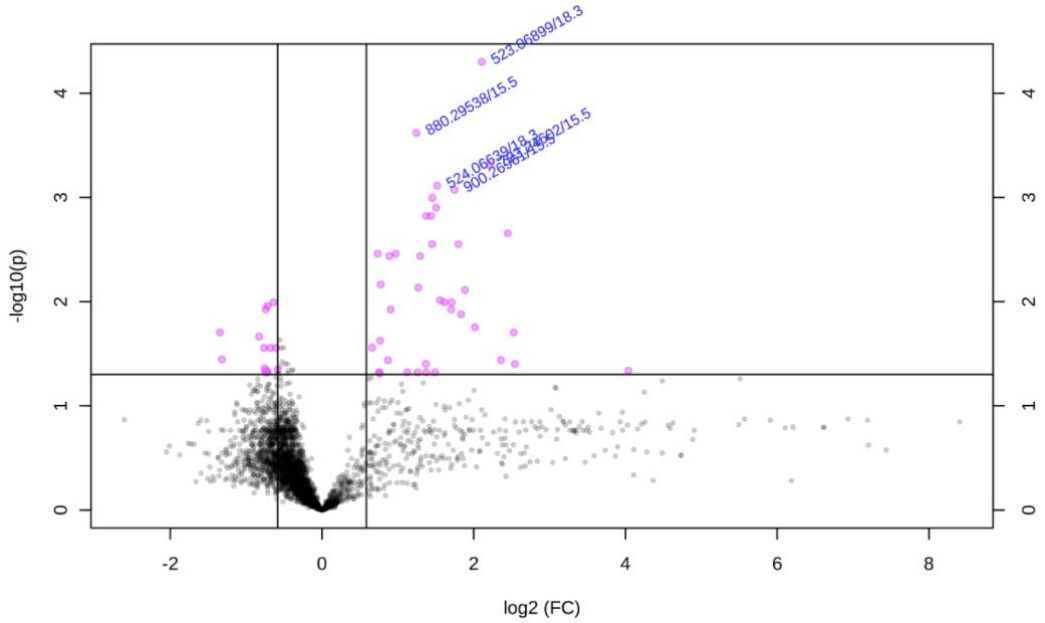


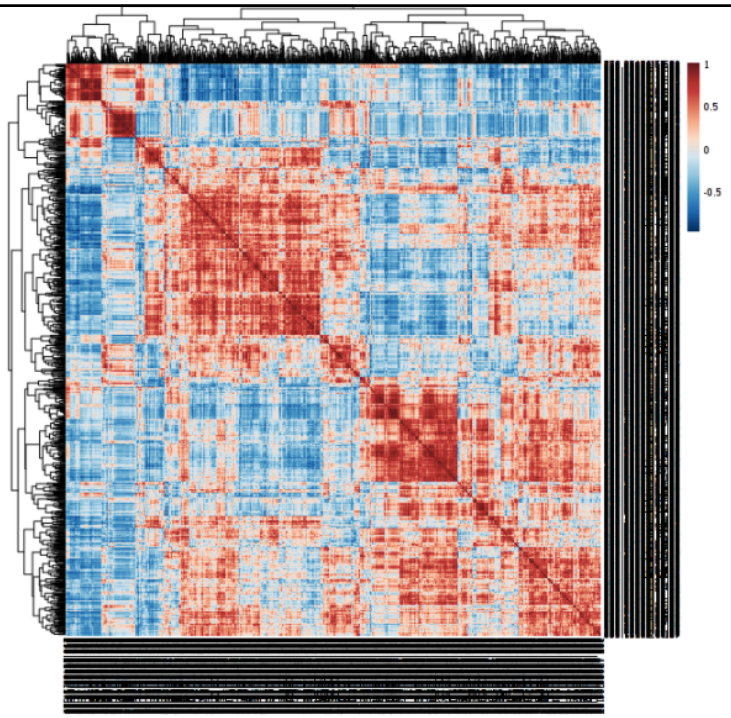
T-test = FDR adjusted





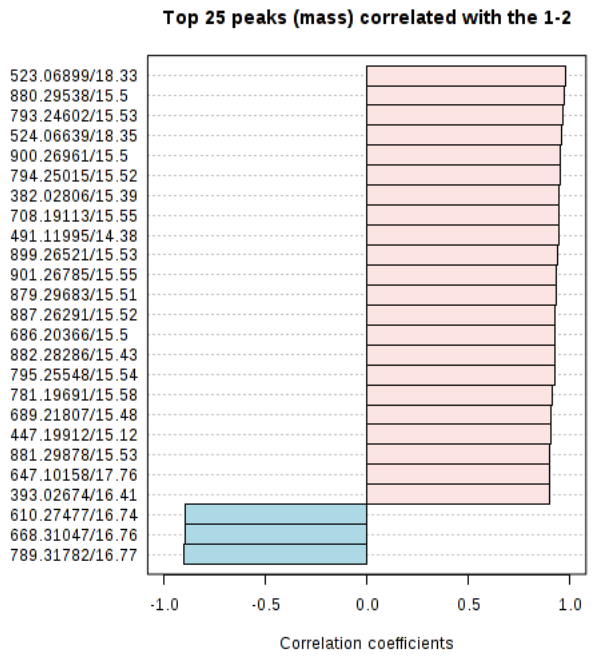
High-resolution Volcano plot





Correlation matrix

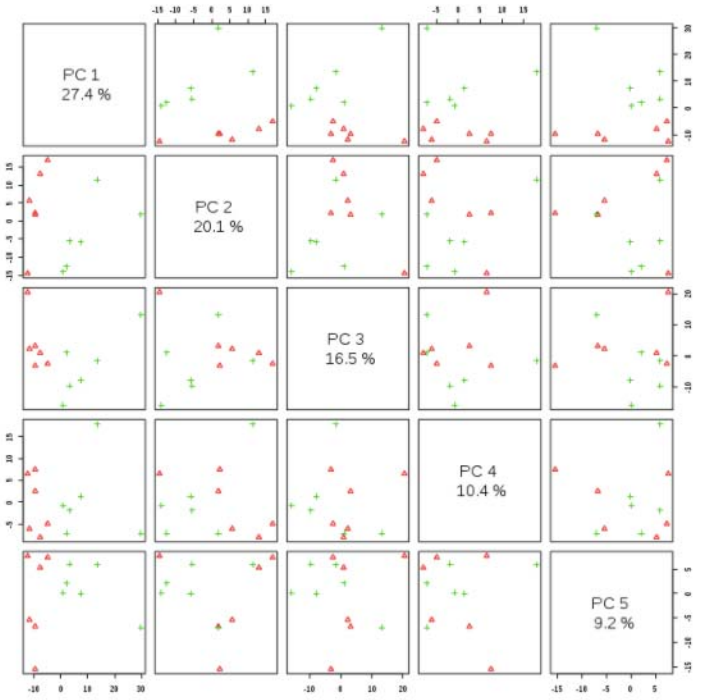
Top features correlated with Genistein vs Control

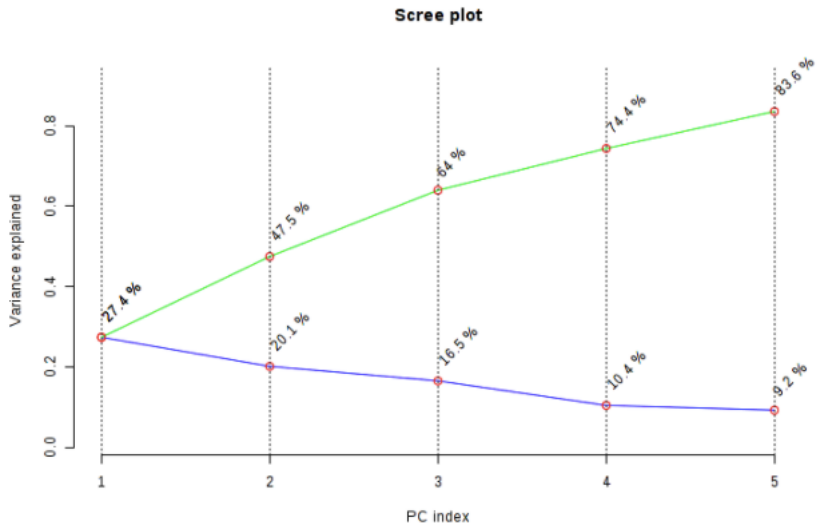


Multivariate analyses

Principal Components Analysis (PCA)

Plots of 5 principal components, taking two at a time.

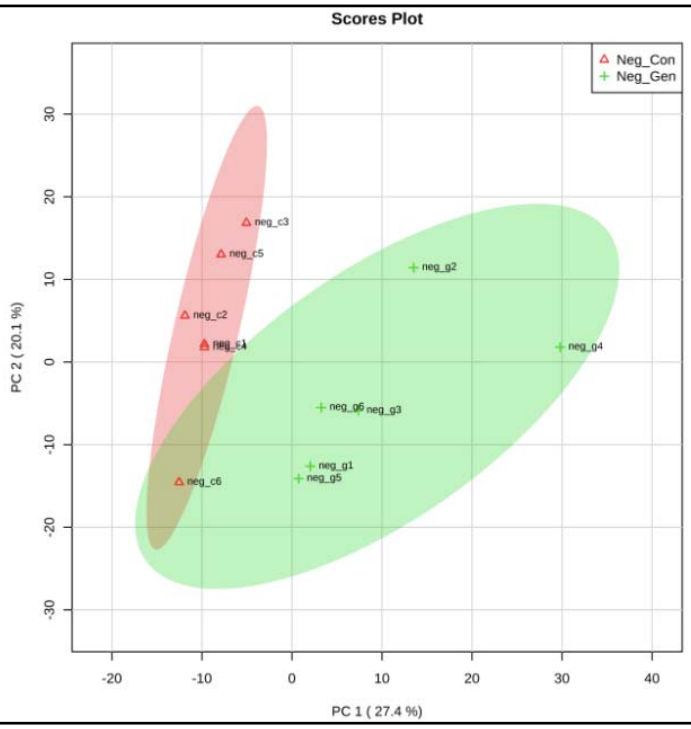




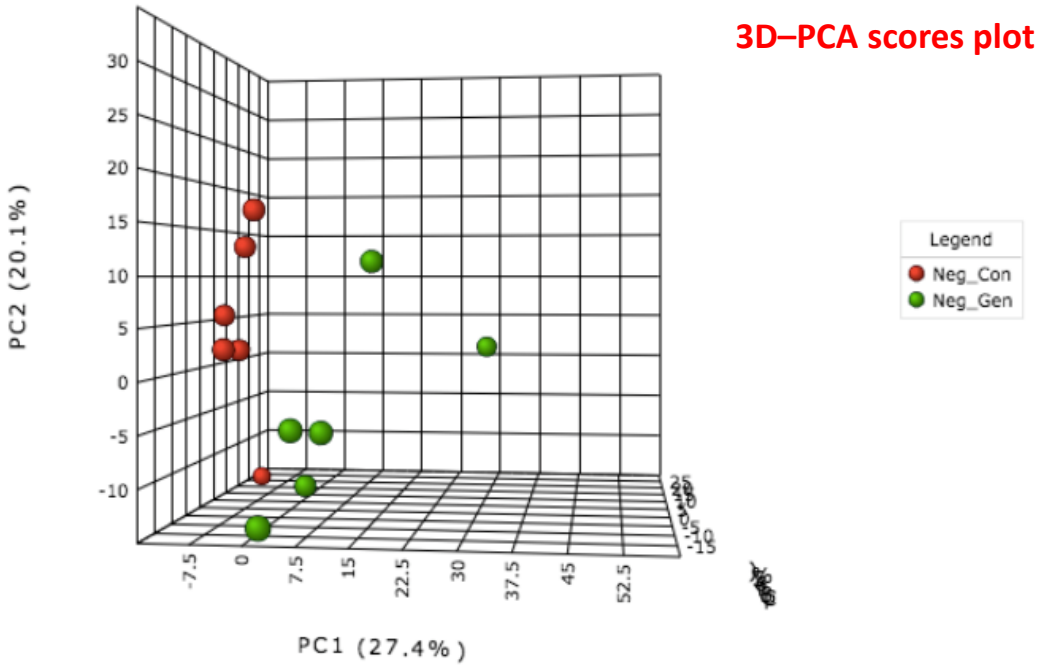
Variation explained by the components

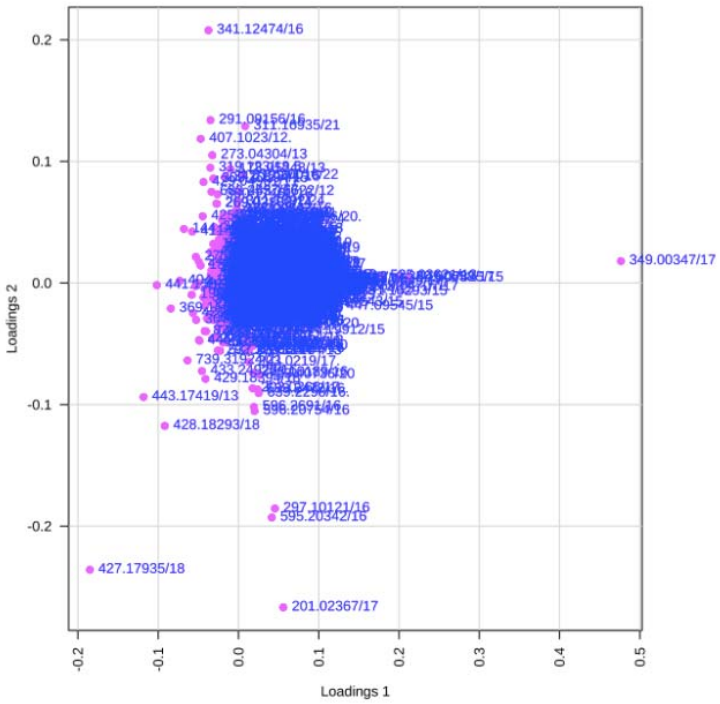
Principal components analysis (PCA) – components 1 and 2

This analysis is unsupervised

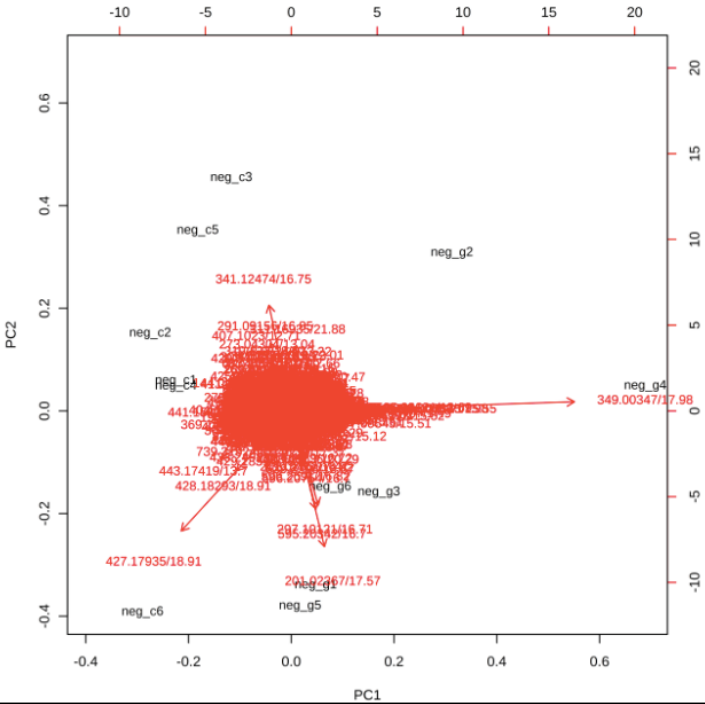


3D–PCA scores plot



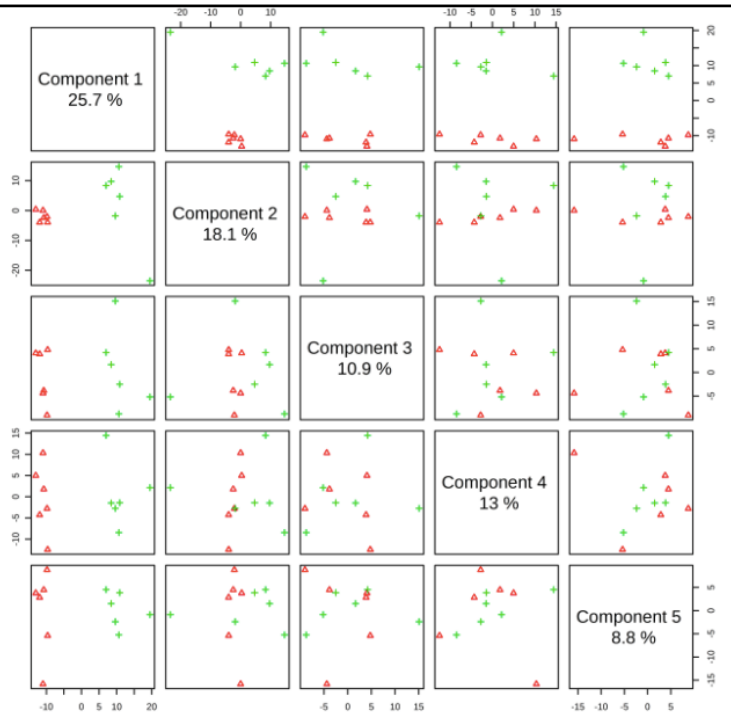


PCA loadings plot

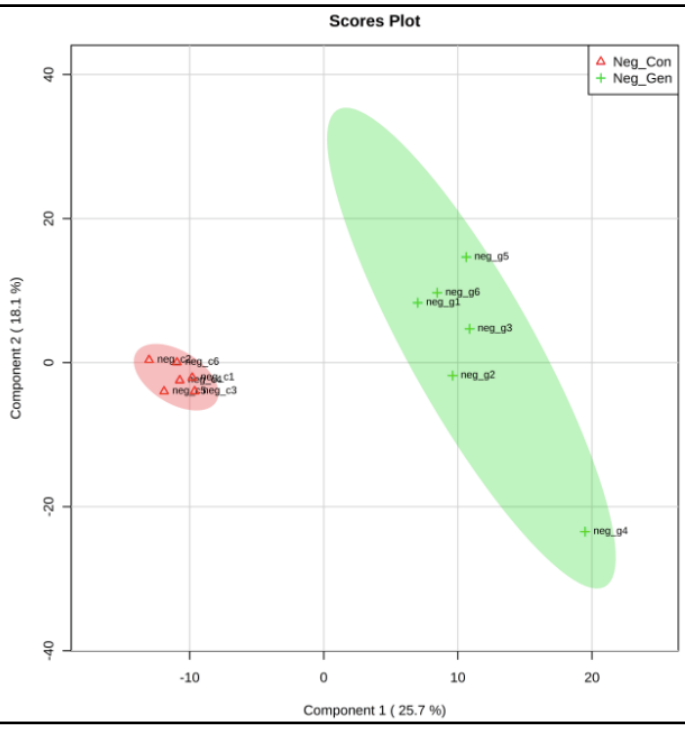


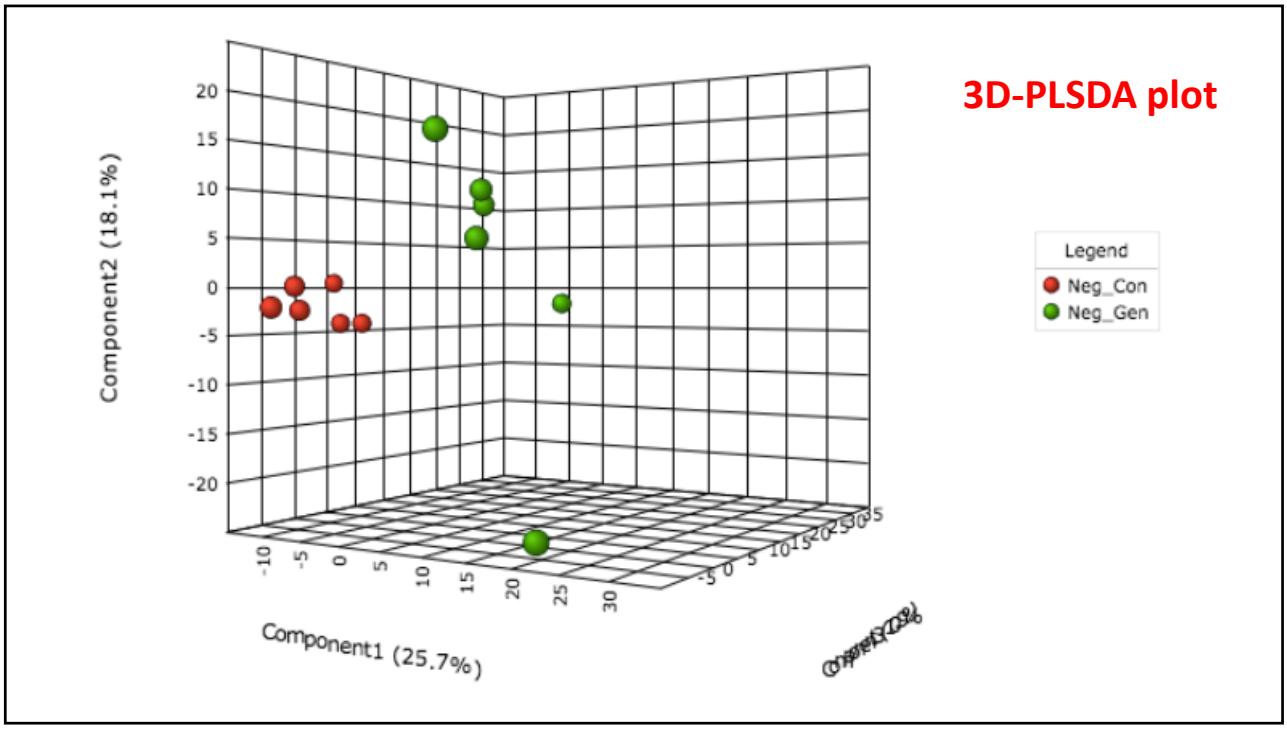
PCA biplot

Partial Least Squares Discriminant Analysis (PLSDA)

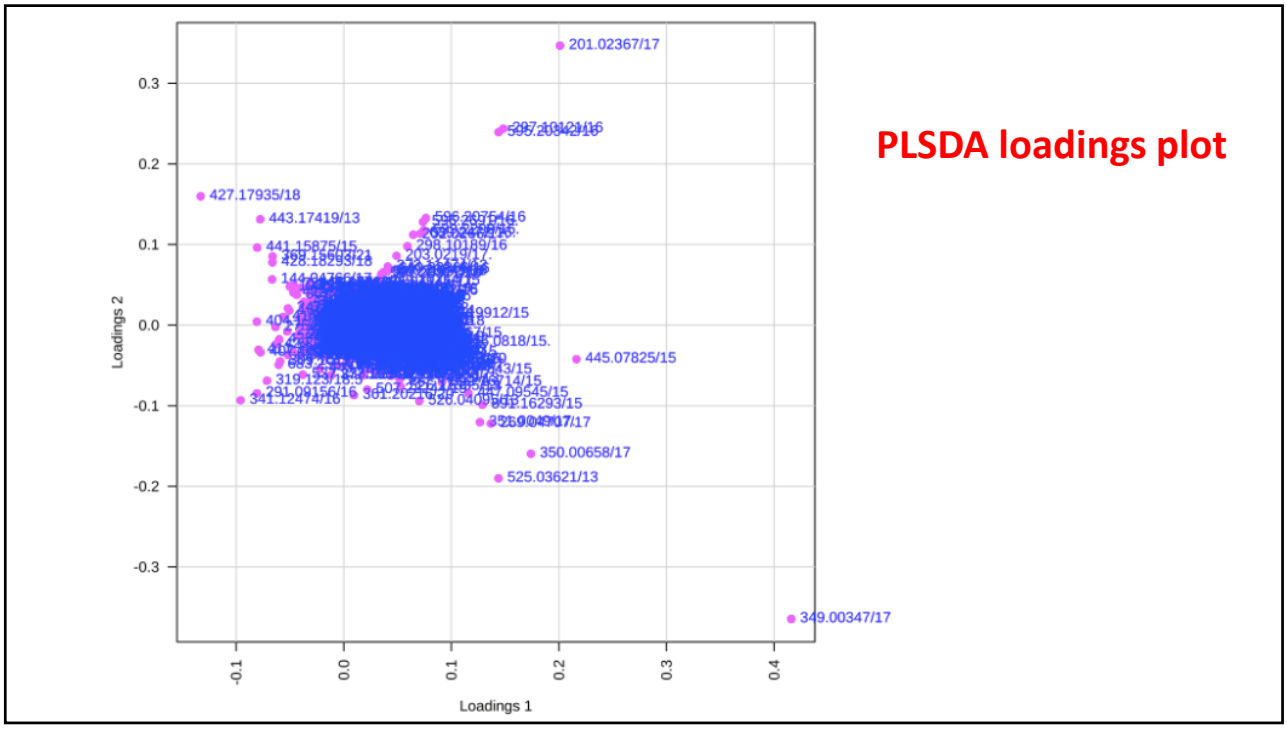


2D-PLSDA plot

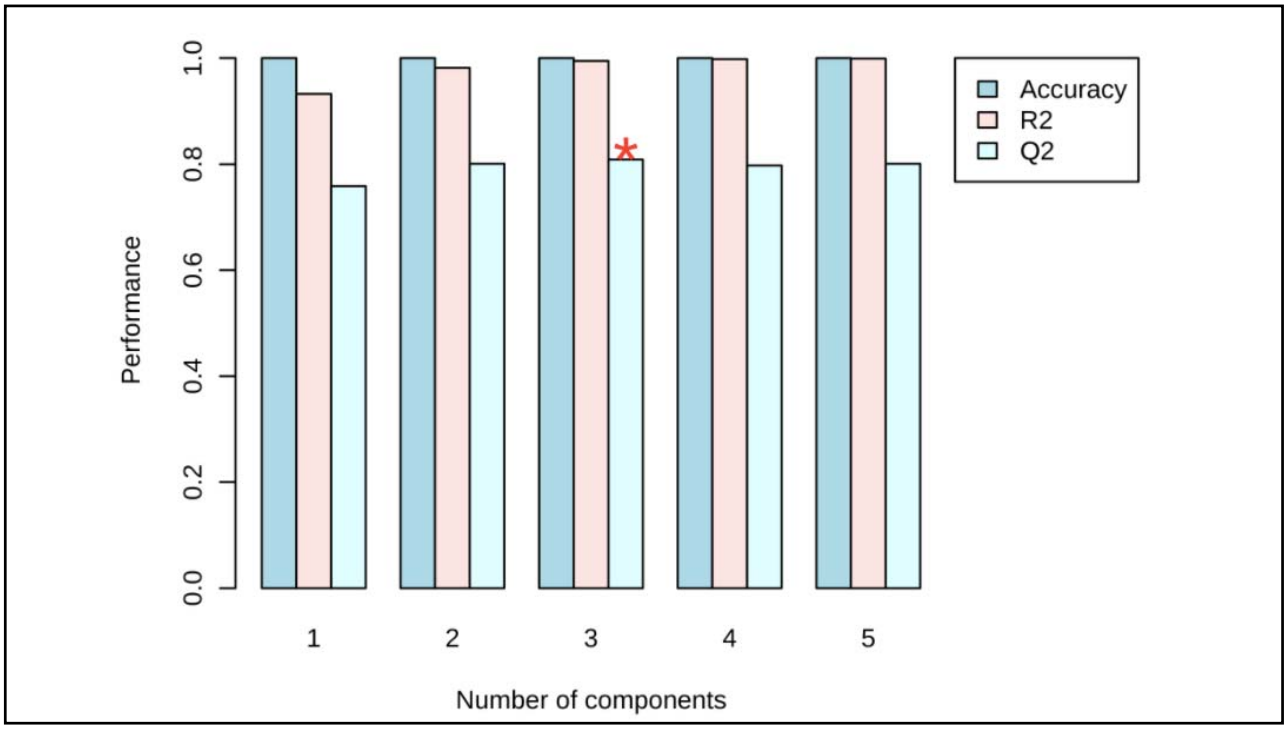


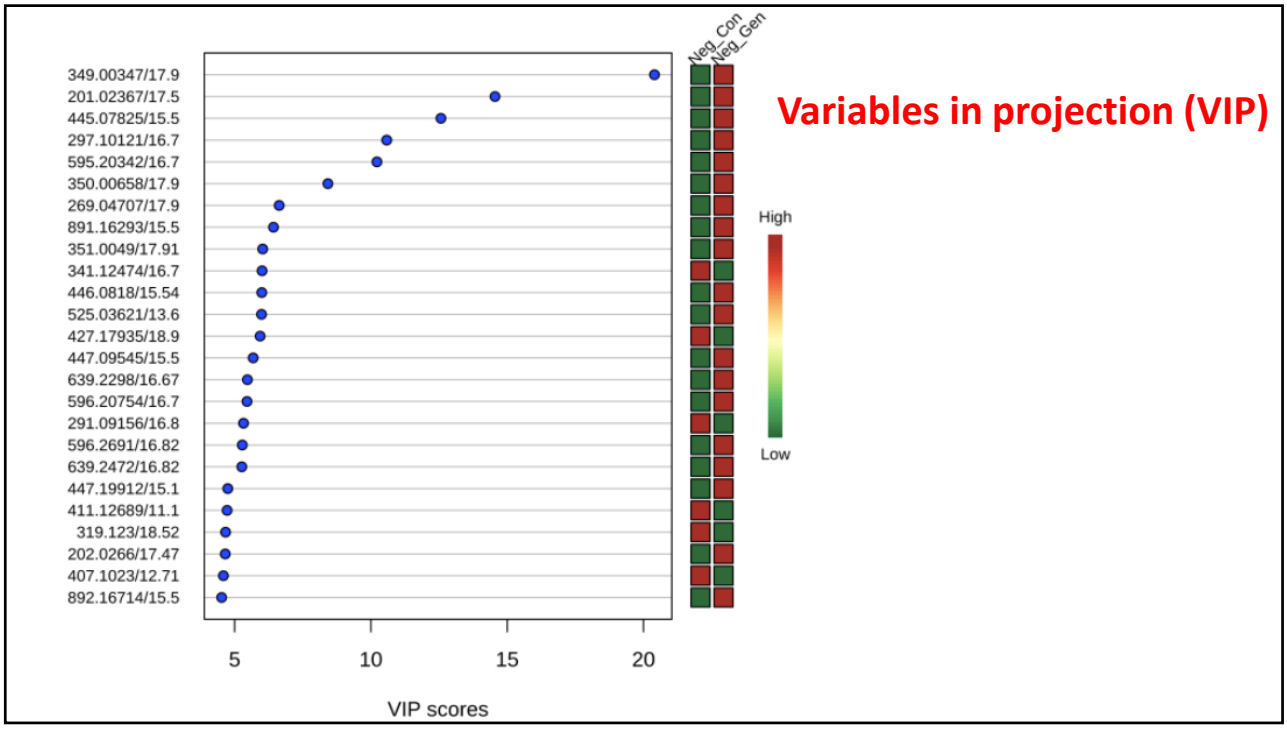


3D-PLSDA plot

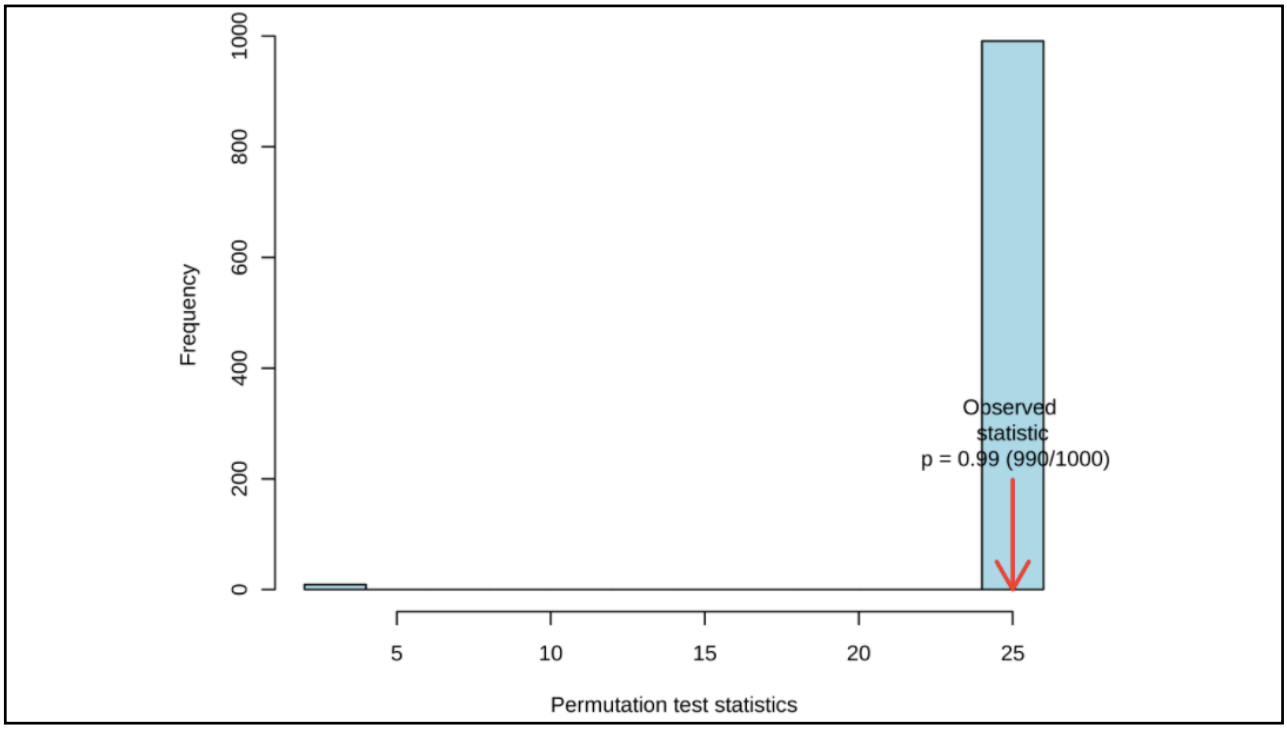


PLSDA loadings plot



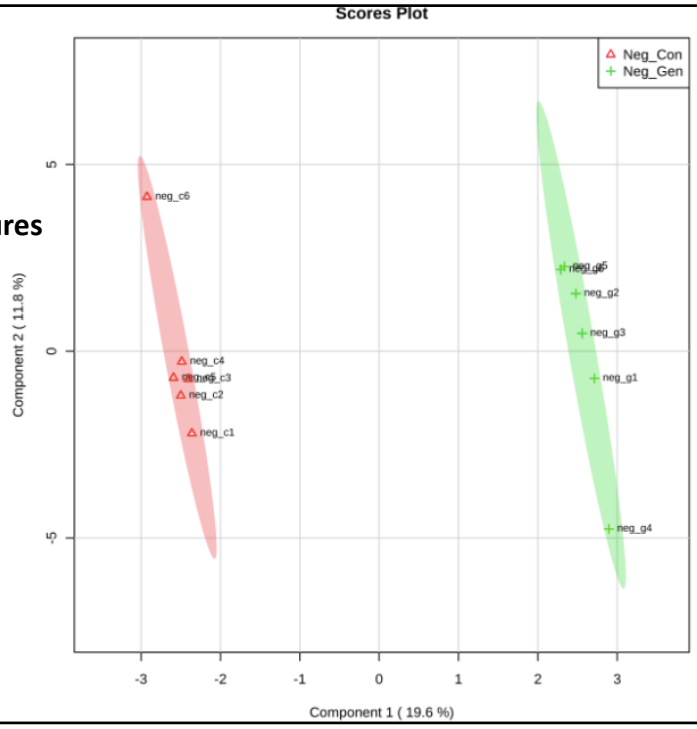


Variables in projection (VIP)

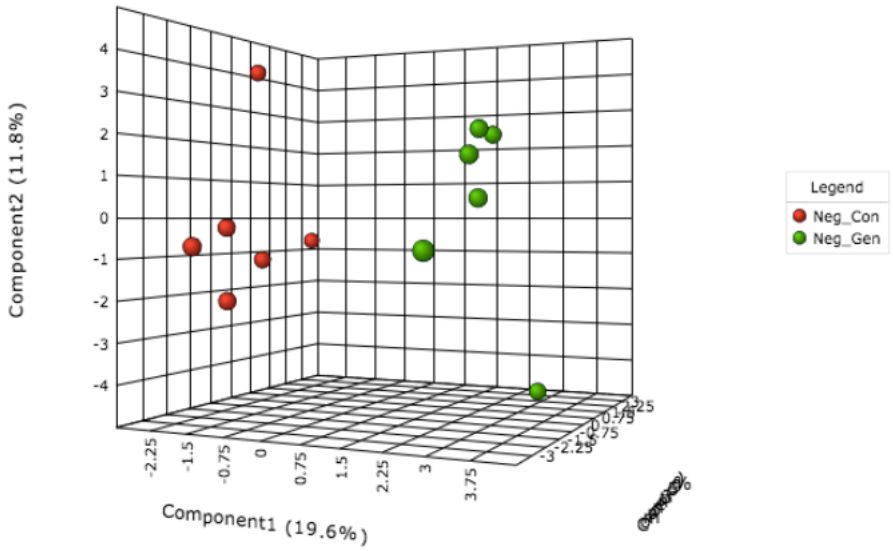


Sparse PLSDA (sPLSDA)

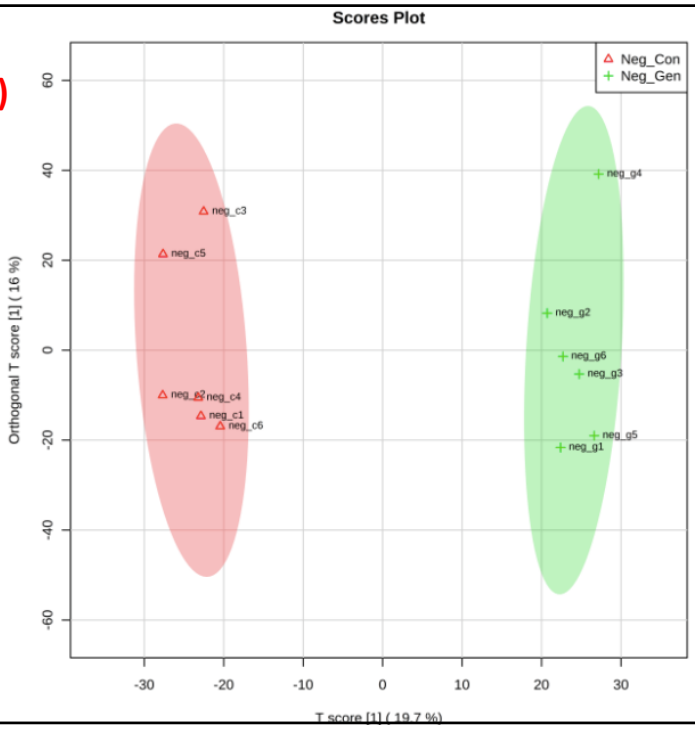
Top ten most significant ion features

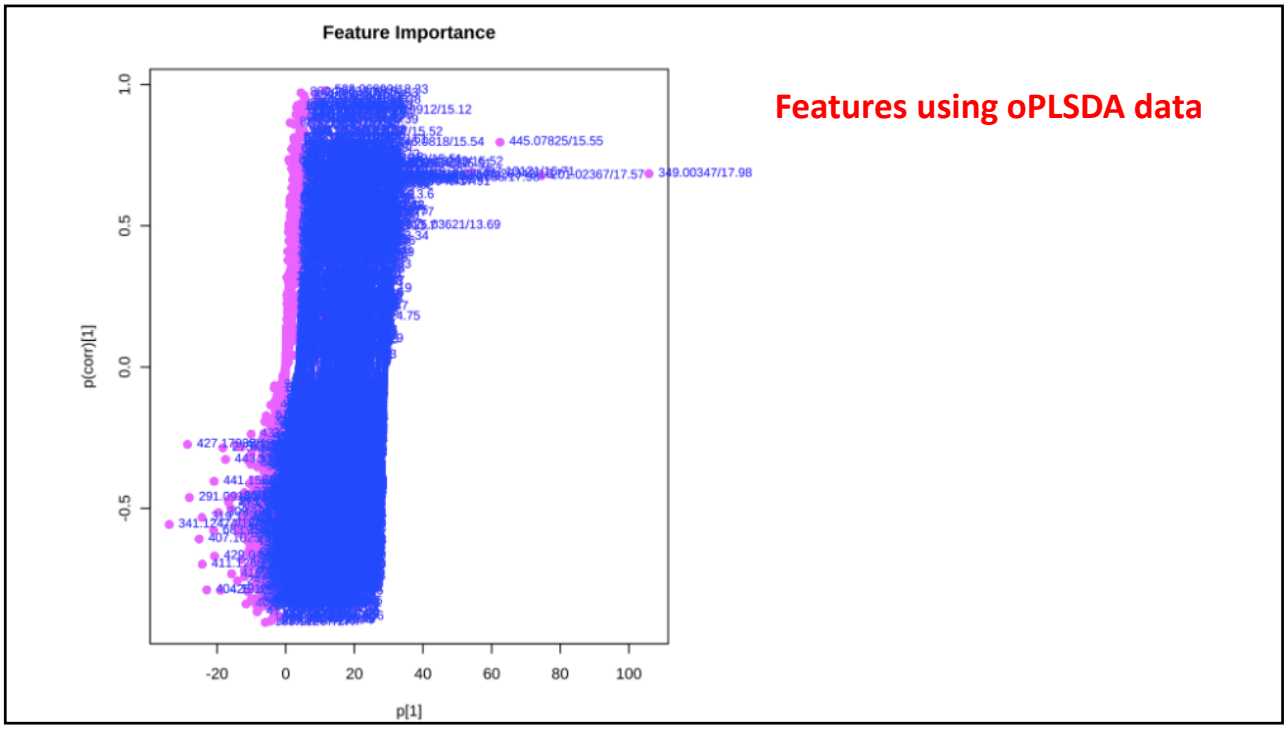


3D-sPLSDA plot

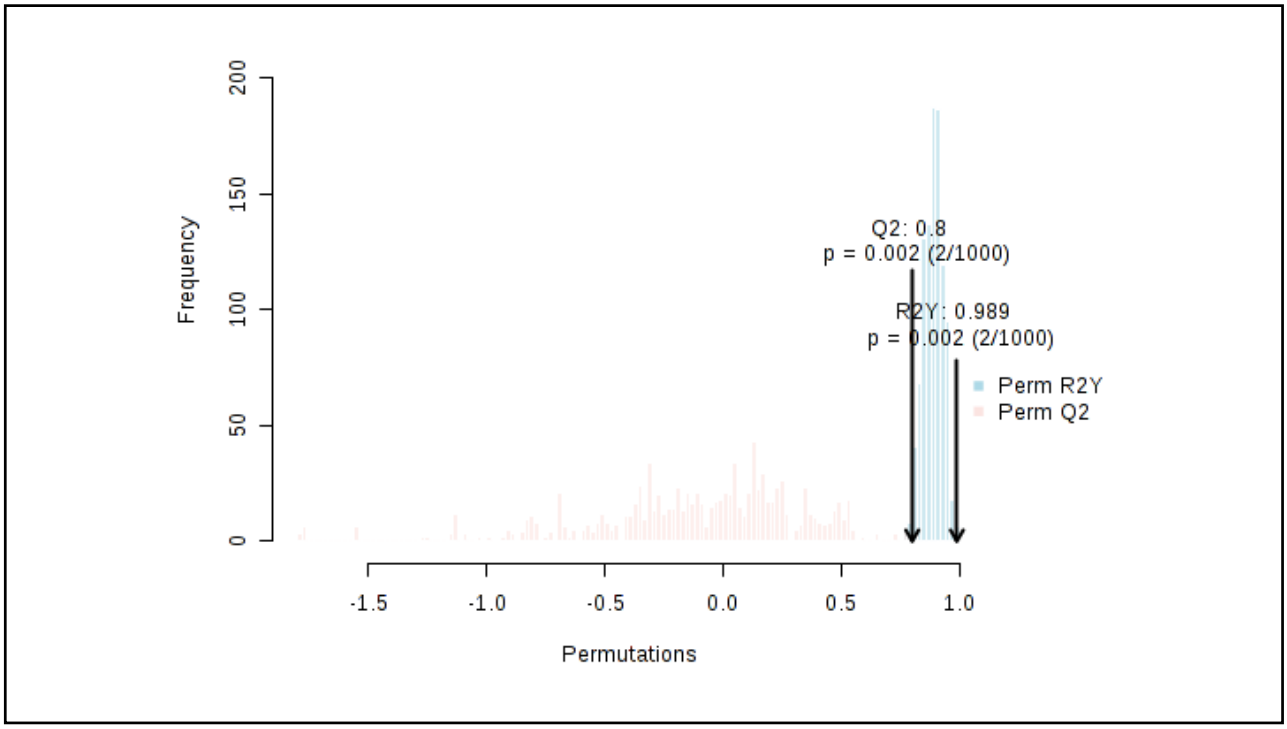


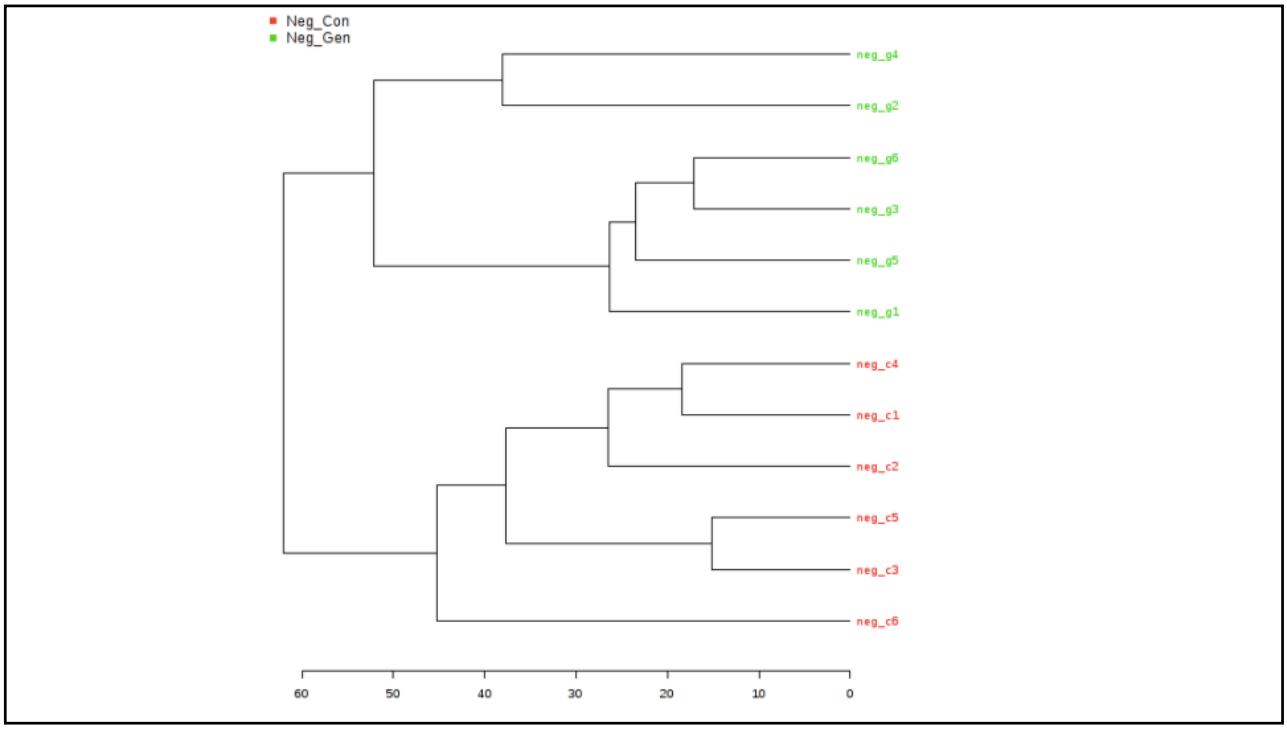
Orthogonal PLSDA (oPLSDA)

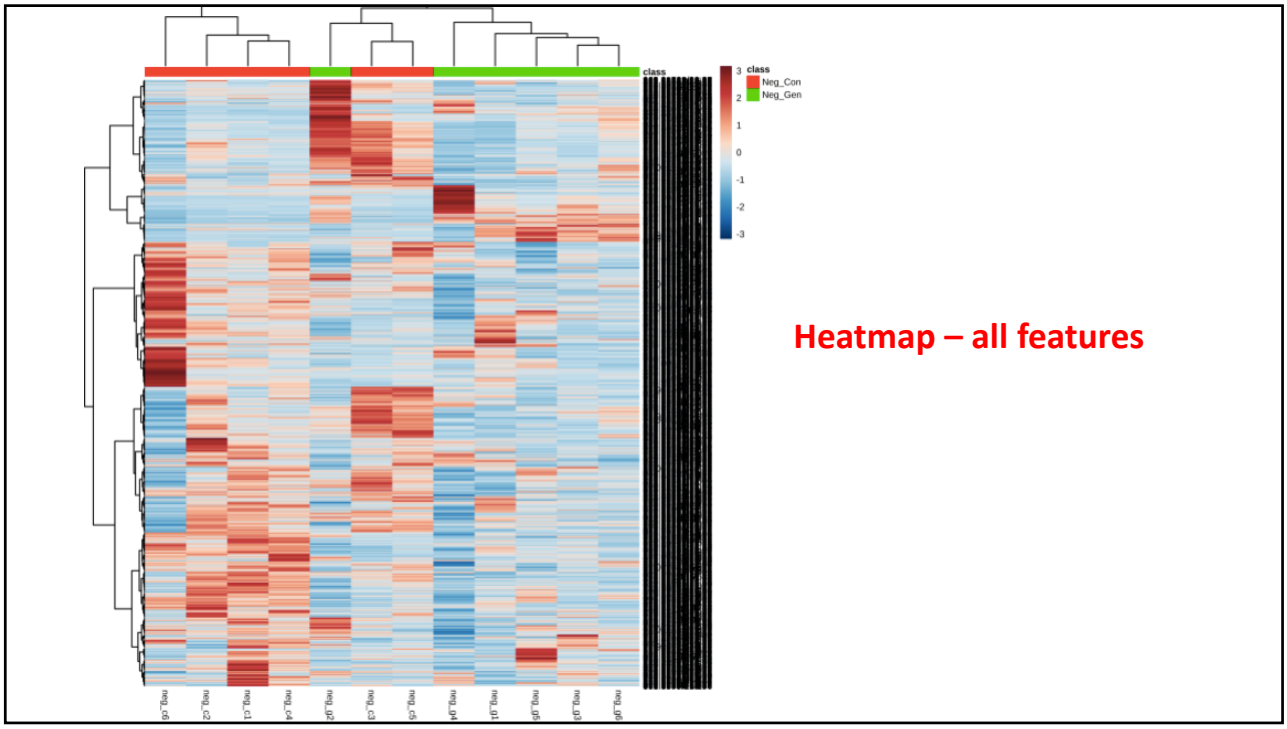




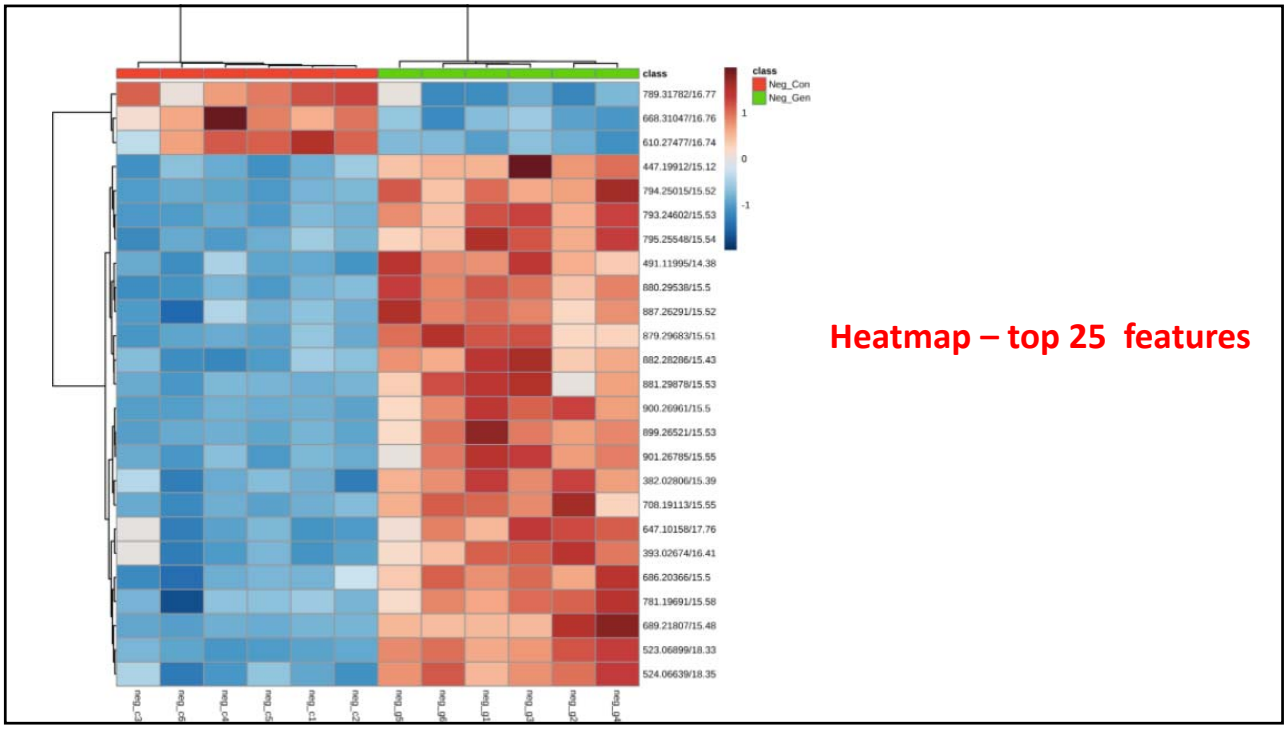
Features using oPLSDA data



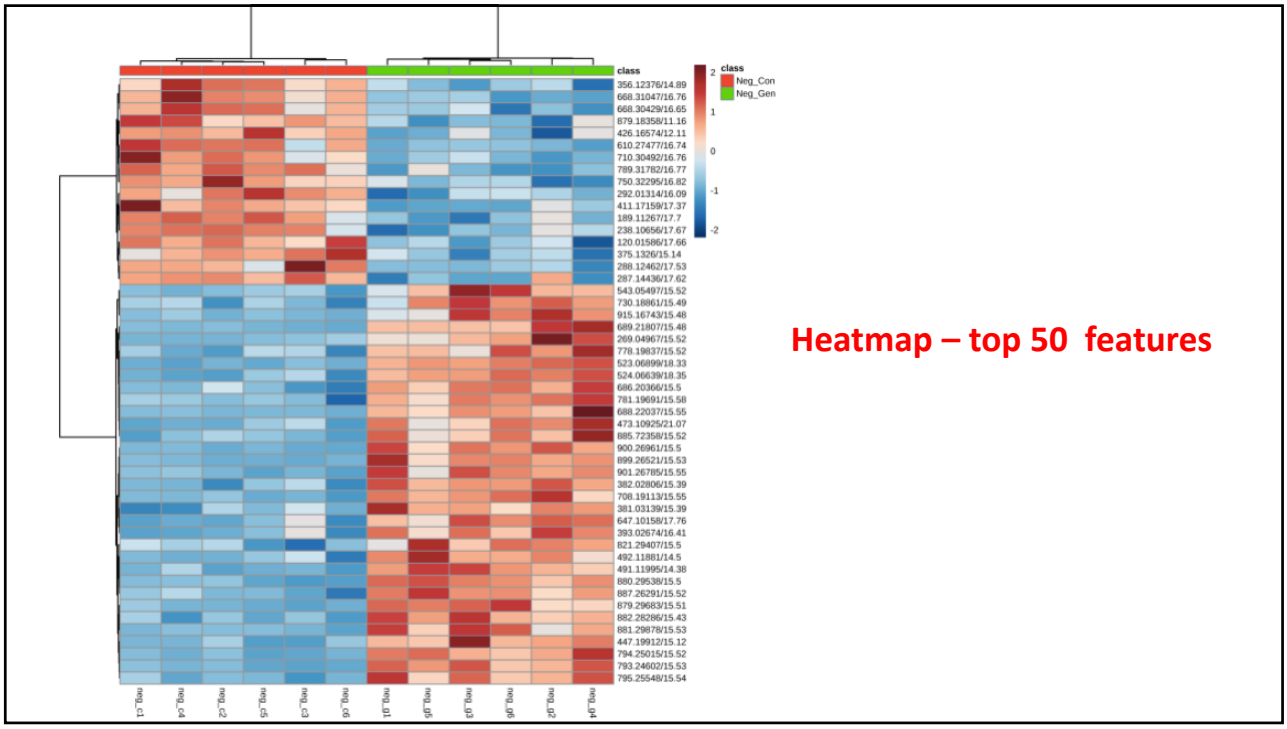




Heatmap – all features



Heatmap – top 25 features



Heatmap – top 50 features

Top 50 features in the VIP

m/z	RT	Comp. 1
349.0035	17.98	20.402
201.0237	17.57	14.552
445.0783	15.55	12.568
297.1012	16.71	10.580
595.2034	16.70	10.221
350.0066	17.98	8.422
269.0471	17.90	6.636
891.1629	15.52	6.426
351.0049	17.91	6.030
341.1247	16.75	6.007
446.0818	15.54	5.997
525.0362	13.69	5.988
427.1794	18.91	5.936
447.0955	15.51	5.680
639.2298	16.67	5.469
596.2075	16.70	5.455
291.0916	16.85	5.327
596.2691	16.82	5.281
639.2472	16.82	5.264
447.1991	15.12	4.749
411.1269	11.14	4.724
319.1230	18.52	4.669
202.0266	17.47	4.657
407.1023	12.71	4.589
892.1671	15.52	4.525
404.1916	13.38	4.404
298.1019	16.72	4.217
893.1754	15.51	4.098
429.0496	11.92	3.962
441.1588	15.05	3.866
275.0969	18.54	3.804
683.2557	16.74	3.791
309.1019	15.43	3.704
425.1785	16.68	3.618
443.1742	13.70	3.560
203.0219	17.37	3.547
823.2609	11.13	3.416
640.2337	16.67	3.143
269.0497	15.52	3.131
415.1972	19.11	3.097
640.2685	16.84	3.001
428.1829	18.91	2.980
380.1746	16.69	2.975
373.1147	13.60	2.935
526.0410	13.70	2.914
537.2335	18.41	2.900
269.0478	20.56	2.879
273.0430	13.04	2.852
369.1560	21.45	2.838
144.0477	17.12	2.745

m/z	RT	Comp. 1
144.0477	17.12	2.745
186.1152	17.75	2.582
187.0829	16.87	2.624
198.1149	18.69	2.340
201.0237	17.57	14.552
202.0266	17.47	4.657
203.0219	17.37	3.547
204.0679	16.05	2.058
214.1105	17.43	2.034
242.1407	14.95	2.595
269.0211	14.06	2.549
269.0388	14.03	2.486
269.0471	17.90	6.636
269.0478	20.56	2.879
269.0497	15.52	3.131
270.0494	17.90	2.723
273.0430	13.04	2.852
275.0969	18.54	3.804
291.0916	16.85	5.327
292.0935	16.88	2.121
293.0992	17.00	2.004
297.1012	16.71	10.580
298.1019	16.72	4.217
307.0770	17.22	2.037
309.1019	15.43	3.704
317.1071	18.45	2.021
319.1230	18.52	4.669
320.1281	18.49	2.092
337.1327	15.13	2.341
337.1331	16.70	2.245
341.1247	16.75	6.007
342.1284	16.73	2.571
349.0035	17.98	20.402

349.0035	17.98	20.402
350.0066	17.98	8.422
351.0049	17.91	6.030
352.0058	18.07	2.334
367.1413	20.65	2.178
369.1560	21.45	2.838
373.1147	13.60	2.935
380.1746	16.69	2.975
404.1916	13.38	4.404
405.1933	13.37	2.210
407.1023	12.71	4.589
408.1059	12.69	2.001
411.1269	11.14	4.724
412.1296	11.14	2.135
415.1972	19.11	3.097
425.1642	12.09	2.352
425.1652	18.41	2.394
425.1785	16.68	3.618
427.1794	18.91	5.936
428.1829	18.91	2.980
429.0496	11.92	3.962
432.2197	16.48	2.112
433.0793	10.75	2.258
433.2049	15.50	2.076
433.2492	16.49	2.319
435.2224	15.30	2.019
441.1588	15.05	3.866
443.1742	13.70	3.560
445.0783	15.55	12.568
446.0818	15.54	5.997
447.0955	15.51	5.680
447.1991	15.12	4.749
449.1075	15.77	2.706

513.0725	13.83	2.345
523.0690	18.33	2.267
525.0362	13.69	5.988
526.0410	13.70	2.914
526.1134	13.34	2.114
527.0433	13.70	2.157
537.2335	18.41	2.900
587.3044	17.35	2.039
595.2034	16.70	10.221
596.2075	16.70	5.455
596.2691	16.82	5.281
597.2109	16.70	2.652
597.2637	16.82	2.517
621.1138	12.61	2.152
639.2298	16.67	5.469
639.2472	16.82	5.264
640.2337	16.67	3.143
640.2685	16.84	3.001
668.1241	15.50	2.634
668.6207	15.51	2.212
675.2739	16.80	2.249
675.3014	16.75	2.277
683.2557	16.74	3.791
684.2595	16.74	2.322
739.3192	21.46	2.186
767.3151	16.74	2.267
823.2609	11.13	3.416
824.2636	11.13	2.078
891.1629	15.52	6.426
892.1671	15.52	4.525
893.1754	15.51	4.098
894.1822	15.52	2.461