

Bioinformatic and statistical approaches for high-throughput lc-ms data

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Abstract

Comprehensive data analyses for high-throughput lc-ms data are presented. Methods of statistical analysis and integration for multifactorial experiments are shown. Examples data sets comes from studies on cereals response to pathogen infection and barley (*Hordeum vulgare*) under drought stress. Primary metabolites, secondary metabolites and proteins were analyzed.

Data preprocessing, analysis and visualization was done in the R system. The statistical analyses were performed using procedures in Genstat package. Methods of omic data integration and visualization by networks are presented.

The correlation networks and differential correlation networks were constructed to compare relations between metabolites and proteins under different conditions. Traits are represented by nodes, lines (edges) correspond to correlations between the pairs of traits. Modules - clusters with highly correlated traits are detected. Hubs, which are traits with many connections (correlations with other traits) are indicated.

Correlation network analysis was done using WGCNA package in R, the Pearson correlation matrix was transformed into an adjacency matrix using a power function. Modules were detected by clustering. Differential correlation networks were created using the test based on Fisher's Z transformation, with Bonferroni correction. Visualization of networks was performed in Cytoscape.

The algorithms can be adapted to any high-throughput lc-ms data.

Biography:

Aneta Sawikowska completed her Ph.D. thesis under supervision of world-class professor Charles Johnson (William & Mary, Williamsburg, USA). She completed an internship at The James Hutton Institute, Dundee, United Kingdom. She gained years of experience in data analysis working for 10 years as an assistant professor at the Institute of Plant Genetics of the Polish Academy of Sciences in Poznań. From 2016, an assistant professor at the Department of Mathematical and Statistical Methods at the University of Life Sciences in Poznań. Author of 22 publications in the field of bioinformatics, statistical analysis of metabolomic, phenotypic and lipid data, repeatedly using R.

Speaker Publications:

- 1."Phenolic Metabolites from Barley in Contribution to Phenome in soil Moisture Deficit", International Journal of Molecular Sciences/ Volume 21, Issue 17, 21 August 2020
2. "In search of biomarkers and the ideotype of barley tolerant to water scarcity", International Journal of Molecular Sciences/ Volume 21, Issue 17, 21 August 2020
3. "Covariance regularization for metabolomic data on the drought resistance of barley", Biometrical Letters/Volume 56: Issue 2, 16 Dec 2019
4. "Silver nanoparticles affect phenolic and phytoalexin composition of *Arabidopsis thaliana*", Science of The Total Environment /Volume 716, 10 May 2020, 135361
- 5."Proteomic analysis of barley mapping population subjected to drought identifies proteins with genotype×environment interaction and pQTLs", September 2019

[10th World Congress on Chromatography](#); April 16-17, 2020 -Webinar

Abstract Citation:

Aneta Sawikowska, Bioinformatic and statistical approaches for high-thoughtput lc-ms data, Chromatography 2020, 10th World Congress on Chromatography; April 16-17,2020- Webinar (<https://chromatography.conferenceseries.com/abstract/2020/bioinformatic-and-statistical-approches-for-high-thoughtput-lc-ms-data>)

