Metabolite AutoPlotter - an application to automatically process and visualise metabolite data in the web-browser

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Abstract

Background Metabolomics is gaining popularity as a standard tool for the investigation of biological systems. Yet, parsing metabolomics data in the absence of in-house computational scientists can be overwhelming and time consuming. As a consequence of manual data processing the results are often not processed in full depth, so potential novel findings might get lost.

Methods To tackle this problem we developed Metabolite AutoPlotter, a tool to process and visualise metabolite data. It reads as input pre-processed compound-intensity tables and accepts different experimental designs, with respect to number of compounds, conditions and replicates. The code was written in R and wrapped into a shiny-application that can be run online in a web-browser on https://mpietzke.shinyapps.io/autoplotter.

Results We demonstrate the main features and the ease of use with two different metabolite datasets, for quantitative experiments and for stable isotope tracing experiments. We show how the plots generated by the tool can be interactively modified with respect to plot type, colours, text labels and the shown statistics. We also demonstrate the application towards 13-C-tracing experiments and the seamless integration of natural abundance correction, which facilitates the better interpretation of stable isotope tracing experiments. The output of the tool is a zip-file containing one single plot for each compound as well as sorted and restructured tables that can be used for further analysis.

Conclusion With the help of Metabolite AutoPlotter it is now possible to automate data processing and visualisation for a wide audience. High quality plots from complex data can be generated in a short time with pressing a few buttons. This offers dramatic improvements over manual processing. It is significantly faster and allows researchers to spend more time interpreting the results or to perform follow-up experiments. Further this eliminates potential copy-and paste errors or tedious repetitions when things need to be changed. We are sure that this tool will help to improve and speed up scientific discoveries.

Full-text

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