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Isotope labeling-assisted metabolomics: Novel workflows for improved LC-HRMS based research

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Stable isotope labeling techniques are becoming increasingly used in numerous MS based metabolomic studies. The use of stable isotope labeled tracers and labeled biological samples are well suited to tackle major obstacles of untargeted metabolomics such as the elucidatation of global biochemical composition of biological samples, the study of tracer metabolisation or to improve quantification by internal standardisation.

In this study we present novel LC-HRMS based, labeling-assisted workflows and data processing tools (MetExtract and FragExtract) for the untargeted profiling of biological samples and MS/MS spectrum elucidation. The presented approaches involve the measurement of mixtures of ^{13}C labeled and non-labeled biological samples or tracer metabolites. For global metabolomecharacterisation and untargeted profiling of tracer metabolisation, a two dimensional data filtering is performed. First every mass spectrum is inspected for labeling specific MS signal patterns to only extract truly biology derived metabolite ions. Subsequently, MetExtract performs chromatographic peak picking using a wavelet implementation and predicts feature groups to convolute different adducts and in-source fragments of the same metabolite. The resulting data matrix does not only form a reliable basis for metabolite annotation and further statistical analysis but is also excellently suited for evaluating the performance of the complete analytical workflow.

A detailed description of the workflow concepts is given and their performance and limitations are discussed. The complete workflows are exemplified with selected biological studies on the characterization of the metabolome of the fungus *Fusarium graminearum* and wheat, and the untargeted profiling of mycotoxins in wheat as well as phenylalanine in grapevine.

Biography

Rainer Schuhmacher is Associate Professor at the University of Natural Resources and Life Sciences, Vienna (BOKU) where he is heading the working group Metabolomics and Bioactive Compounds. Recently, his research focus has shifted from target analytics towards LC-MS and GC-MS based metabolomics of microbes and plants with a special focus on the interaction between living organisms. He received his degrees in Chemistry from the University of Konstanz, Germany and the Vienna University of Technology and in 2009. He earned his habilitation in Analytical Chemistry from the BOKU University. He is (co-)author of more than 80 SCI publications.

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