

Isotope labeling-based plant metabolite analysis using high resolution FT-ICR MS

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Distinguishing biological from non-biological peaks in mass spectrometry-based metabolome analysis is a well known problem for metabolomics. To overcome this problem a new strategy for fast and high resolution metabolite profiling based on the combination of Fourier Transform Ion Cyclotron Resonance Mass Spectrometry and ^{13}C -isotope labelling of entire metabolomes will be discussed and presented. The strategy, which is based on the pair-wise comparison of chemical formulas identified from metabolite extracts of *Arabidopsis thaliana* plants grown under identical conditions but with different, namely $^{12}\text{CO}_2$ or $^{13}\text{CO}_2$, carbon sources, not only allows to clearly discriminate biological from non-biological compounds in the extracts, but also to achieve quantitative information of the measure compounds.

For this purpose a high resolution LTQ FT Ultra mass spectrometer was used to generate accurate mass fingerprints (mass accuracy < 1ppm) of soluble metabolites from ^{12}C and ^{13}C *Arabidopsis* metabolomic extracts. Thousands of masses from these profiles were then searched, using an in-house developed database search tool, against the calculated, accurate ^{12}C and ^{13}C masses of the publicly available PubChem database.

Applying this strategy to metabolite extracts of *Arabidopsis thaliana* resulted not only in the reproducible identification of 1,024 unambiguous chemical sum formulas, but also in the possibility to relatively quantify a large number of compounds between samples, if ^{13}C metabolite spiking is used for a whole experimental set.

Additionally the differential analysis of the dataset allowed for the prediction of thus far un-described chemical compounds and possible pathways in *Arabidopsis thaliana*, based on the accumulation of unambiguously identified chemical formulas, in specific pathways described for other organisms. Amongst these is an example for a thus far undescribed lysine degradation pathway in *Arabidopsis thaliana*.