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Metabolic profiling by UHR-Q-TOF analysis of dansylated metabolite extracts to study yeast Arginine synthesis mutants

Aiko Barsch[1], Sandy Yates[2], Gabriela Zurek[1], Manhong Wu[3], Bob St. Onge[3], Sundari Suresh[3], Ron Davis[3] and Gary Peltz[3]

[1]Bruker Daltonik GmbH, Bremen, Germany
[2]Bruker Daltonics, Fremont, USA
[3]Stanford University, USA

Many primary polar metabolites, such as amino acids, are poorly retained by reversed phase LC column chemistries which are widely used for untargeted metabolic profiling studies. Dansylation of primary amines, secondary amines and phenolic hydroxyl functional groups in these compounds alters the chromatographic behavior, thus enabling a standard reversed phase (RP)-LC separation with simultaneously enhancement of the signal intensities in electrospray ionization [1].

We analysed dansylated metabolite extracts from yeast wild type and arginine biosynthetic pathway mutants using a novel Ultra high resolution (UHR)-Q-TOF instrument. To prove the hypothesis that upstream or downstream metabolites are altered in abundance in gene knock-out mutants we applied an untargeted Metabolomics workflow.

The identification of metabolites has often been defined as the major bottleneck in Metabolomics research. Confident generation of molecular formulae is the first step in the identification of unknowns. UHR Q-TOF accurate mass and isotopic pattern data from MS and MS/MS spectra can significantly extend the m/z range for reliable formula determinations. The correct molecular formula can subsequently be queried against public databases. Correlating these database matches with information contained in MS/MS spectra enables confirmation of particular structural hypotheses. In this work target compounds could be identified also based on characteristic fragment ions of the dansylated target compounds.

The study revealed an accumulation of precursor metabolites within the arginine biosynthetic pathways before the blocked enzymatic reactions.