DeltaMS: A tool to track isotopologues in GC- and LC-MS data.

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Details

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Abstract

Introduction

Stable isotopic labeling experiments are powerful tools to study metabolic pathways, to follow tracers and fluxes in biotic and abiotic transformations and to elucidate molecules involved in metal complexing.

Objective

To introduce a software tool for the identification of isotopologues from mass spectrometry data.

Methods

DeltaMS relies on XCMS peak detection and X^{13}CMS isotopologue grouping and then analyses

data for specific isotope ratios and the relative error of these ratios. It provides pipelines for recognition of isotope patterns in three experiment types commonly used in isotopic labeling studies: (1) search for isotope signatures with a specific mass shift and intensity ratio in one sample set, (2) analyze two sample sets for a specific mass shift and, optionally, the isotope ratio, whereby one sample set is isotope-labeled, and one is not, (3) analyze isotope-guided perturbation experiments with a setup described in X^{13}CMS.

Results

To illustrate the versatility of DeltaMS, we analyze data sets from case-studies that commonly pose challenges in evaluation of natural isotopes or isotopic signatures in labeling experiment. In these examples, the untargeted detection of sulfur, bromine and artificial metal isotopic patterns is enabled by the automated search for specific isotopes or isotope signatures.

Conclusion

DeltaMS provides a platform for the identification of (pre-defined) isotopologues in MS data from single samples or comparative metabolomics data sets.

Involved units

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Topics

Databases, Web-servers and Prediction Tools

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