

Background/Objective

Orbitrap mass spectrometry (MS) in full scan mode enables the simultaneous detection of hundreds of metabolites and their isotope-labeled forms. Yet, quantitative analysis is challenging since sensitivity is limited for many metabolites, including low-concentration species, poor ionizers, and low-fractional-abundance isotope-labeled forms in isotope-tracing studies. Selected ion monitoring (SIM) is a method to enrich the targeted metabolites and enhance sensitivity. To date, the literature lacks a comprehensive evaluation of the utility of SIM for metabolomics. Here, we investigated using SIM to enhance sensitivity using metabolites from an organic acid-producing *Issatchenkia orientalis* yeast strain.

Approach

Metabolites were extracted from wild type *I. orientalis* SD108 grown in a flask and enriched in the orbitrap analyzer by using the quadrupole as a mass filter to select particular ions (SIM method). Ten metabolite ions of low intensity in both positive and negative modes were identified. Samples were then run five times in the SIM mode and separately five times in full scan mode. Signal-to-noise ratio (S/N) and relative standard deviations (RSD) were determined to assess quantitative performance.

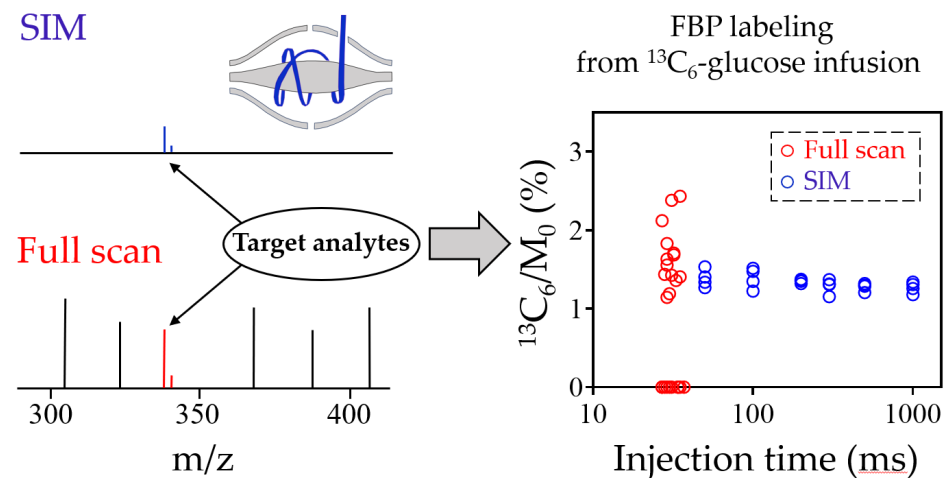
Results

SIM significantly enhanced the detection of ions of low intensity compared to full scan mode, as indicated by improved S/N ratios and measurement precision. In addition, SIM improved the accuracy of isotope-ratio measurements.

Significance/Impacts

Orbitrap MS with SIM enable enhanced metabolome coverage and more accurate quantitation.

Lu et al. 2024. "Selected Ion Monitoring for Orbitrap-Based Metabolomics." *Metabolites* 14: 184. DOI: 10.3390/metabo14040184.



Graphical abstract and comparison of orbitrap MS methods.