

Analyzing microbial whole cell mass spectrum obtained using MALDI-TOF MS not-dedicated for microbial identification

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Abstract

Identifying microbes by weighing species-specific proteins using mass spectrometry has increasingly find use in research, and more importantly, in the clinic. In an approach known as matrix assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS), biomarker proteins such as ribosomal proteins that chronicle the evolutionary divergence of specific species are ionized without fragmentation, and detected with a mass analyzer; thereby, yielding a species-specific mass spectrum. While methodologically sound, practical implementation of the approach encounters two problems: need for a MALDI-TOF MS dedicated for microbial identification (such as Bruker Ultraflex) and a reference library of verified microbe mass spectra. But, what does a non-dedicated MALDI-TOF MS brings to microbial identification? Examination of mass spectra of common bacteria such as *Escherichia coli* DH5 α , *Pseudomonas protegens* Pf-5, *Pseudomonas aeruginosa* PRD-10, and *Bacillus subtilis* NRS-762 obtained using a Bruker Autoflex II MALDI-TOF MS consistently revealed a broad peak around the low mass range which tapered off (with the emergence of a few sharp peaks of high intensity at the higher mass/charge ratio). Such a profile suggests the ionization of a large variety of biomolecules (lipids, carbohydrates, proteins etc.) from the cell surface together with residual nutrient broth that adhered to the cell. To facilitate data analysis, a molecular weight cutoff can be applied to the mass spectrum, which when reconstructed would yield a cleaner view of the types of biomolecules of high abundance that helps inform the identity of an unknown microbe. Looking further, automated data analysis algorithm could be developed to facilitate the above step digitally, while ensuring the relevant peaks for genus identification, i.e., ribosomal proteins, remain firmly within view of the experimenter; thus, enabling a non-dedicated instrument to be utilized for coarse microbial identification. Collectively, mass spectra from MALDI-TOF MS not-dedicated for microbial identification would require post-acquisition data processing to better reveal biomarker peaks useful for coarse (genus level) identification of microbes. But, better instrumentation tuned for ionizing biomolecules and dedicated mass spectra analysis software meant that a mass spectrometer designed for identifying microbes delivers a significant leap in performance in allowing species and even strain level identification useful for informing clinical decisions.

Keywords: MALDI-TOF MS, microbial identification, mass spectrum, biomarker peaks, ribosomal proteins, whole cell, lipids, carbohydrates, proteins, taxonomy,

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Conflicts of interest

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