Understanding the chemical basis for the preferential ionization of specific biomolecules in mass spectrometry analysis of microbial cells

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Abstract

Mass spectrometry-enabled microbial identification has successfully demonstrated the feasibility of using profiled biomolecules for identifying microorganisms based on a chemometric or proteome database search approach. However, mechanisms driving the preferential ionization and detection of particular biomolecules in various types of mass spectrometry remain poorly understood. Specifically, mass spectra obtained from different microbial species remain poorly annotated with respect to the specific types of biomolecules accounting for the peaks. For example, while ribosomal proteins are known to be a significant class of biomolecules that could partially account for the profiled mass peaks in mass spectra of microorganisms, other classes of proteins and biomolecules remain poorly annotated. This raises the important question of how different mass spectrometry approaches ionize different types of biomolecules from a cellular matrix. Specifically, mass spectra of microorganisms reveal that only a couple of mass peaks could capture the phylogeny of a species. However, the proteome of a cell is much larger and more complicated, and yet is not fully profiled by different types of mass spectrometry methods. For example, electrospray ionization mass spectrometry (ESI-MS) and matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) could only provide a small snapshot of the entire bacterial proteome. It could be argued that different mass spectrometry methods provide complementary views of a particular proteome. However, the question remains, how do proteins and biomolecules interact with the different sample preparation and mass spectrometry analysis methods for generating an ion cloud for separation in a mass spectrometer? Thus, efforts could be directed towards understanding how different types of proteins could be preferentially ionized by MALDI-TOF MS. Specifically, different reagents could be used to perform chemical pretreatment on the proteome, which would subsequently be analyzed by mass spectrometry. Thus, a correlative map between types of chemical pretreatment used and the corresponding mass spectra could be obtained. Collectively, knowledge gleaned from the research would illuminate the chemical basis by which specific biomolecules are preferentially ionized under particular conditions, which would inform the development of strategies for increasing the subset of biomolecules ionized from a cellular proteome. Such chemical rules would also aid in the interpretation of mass spectra obtained, particularly in understanding the biological context of the experiment. Overall, the key goal of this research is to help answer the question: what is the biological basis and context of the mass spectrum obtained from cells?

Keywords: mass spectrometry, mass spectra, proteome, preferential ionization, biomolecules, electrospray ionization mass spectrometry, matrix-assisted laser desorption/ionization time-of-flight mass spectrometry, microbial cells, biological context, chemical pretreatment,

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Conflicts of interest

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