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Characterization and cross-validation of the association between structural features and mass spectra profiles

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Abstract

Mass spectrometry (MS) has become a standard technique to identify peptides. In tandem mass spectrometry (MS/MS) experiments, the proteins are extracted from the sample and digested. Subsequent ionization produces first precursor and then fragment ions. This process results in a spectra graph relating the intensity of the fragment ions (that indicates the ion abundance) to the mass/charge (m/z) ratio. Peptide and protein identification depends on the ability of the MS/MS technique to detect fragment ions and this is correlated with the intensity recorded in the mass spectra. A methodical identification and validation of sequence structural factors that may influence the ion fragment abundance was undertaken. A robust characterization of the factors was attained by considering a large data set and models that accommodated the interdependence among the ion fragment observations within protein. A total of 61,543 peptides identified based on 6,352,528 ion fragments were considered. The data set was partitioned into 10 independent data sets with comparable distribution of structural factor levels. A stepwise model selection approach was applied and the factors consistently validated across data sets were identified. The structural factors consistently associated with ion fragment intensity included neutral mass loss, proton mobility, the charge and number of Proline and basic residues in the precursor and fragment ion. The identified trends can be used to adjust the spectra profiles. Our findings demonstrate the multidimensional character of fragment ion abundance in mass spectrometry experiments.

Biography

Sandra Rodriguez Zas is a Professor of Bioinformatics in the Departments of Animal Sciences and Statistics at the University of Illinois, Urbana-Champaign. She received her M. Sc. and Ph.D. in Quantitative Genetics from the University of Wisconsin-Madison. She is the director of the Bioinformatics Core of the Proteomics Center for Cell-Cell Signaling at the University of Illinois. Dr. Rodriguez Zas is the chair of the M. Sc. in Bioinformatics program at the University of Illinois and received a fellow appointment from the National Center for Supercomputing. Her research centers on applying advanced statistical and computational tools to further mine proteomic, genomic and transcriptomic experiments and understand the molecular architecture of complex traits in human, biomedical models, and livestock species.