

High mass accuracy and theoretical peptide distributions

Rovshan G. Sadygov

University of Texas Medical Branch, USA

High mass resolution and accuracy of modern mass spectrometers allow for probing structured distribution of experimental precursor mass in large-scale proteomics experiments. The peptide masses are structured with well defined peaks (mass regions densely populated by peptides) and troughs (regions with low peptide densities). For small peptide masses, the troughs contain so called "forbidden zones" - mass regions which do not hold peptide species. As the peptide mass increases, the forbidden zones shrink in size and finally disappear. However, the peak-centered structure of the peptide masses persists for all mass values. The positions of the peak centers evolve on the mass axis, as the distance between the peak centers is about 1.00044 Da on average. We use theoretical peak distributions to model peptide sampling in data-dependent acquisition mode, and phosphopeptide analyses. We introduce a new concept, peak deviation, which is the mass difference from the evolving peak center position. Peak deviations form a well-defined, unimodal distribution. Therefore, sampling of peptides from whole mass axis is modeled by sampling from the peak deviations distribution. When the sample contains species significantly distinct in their mass defects, the distribution of mass deviations reflects this. Applications to publicly available, large-scale phosphoproteome data showed that one can evaluate the phosphoproteome content of a sample solely based on the precursor masses of species.

Biography

Rovshan G. Sadygov has completed his Ph.D. in Physics from M.V. Lomonosov Moscow State University. He did postdoctoral studies at the Johns Hopkins University and the Scripps Research Institute. Currently, he is an Assistant Professor of Bioinformatics at the University of Texas Medical Branch and is a scientist at the Sealy Center for Molecular Medicine. He has published more than 45 papers in peer-reviewed journals and is serving as an editorial board member in bioinformatics and proteomics related journals.

rovshan.sadygov@utmb.edu