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Blind Post-translational Modification Detection via Dynamic Time Warping Algorithm Based Database Search

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Abstract

The indentation of Post-translational Modifications (PTMs) is a challenging problem in protein identification. Recently, our group introduced a dynamic time warping (DTW) algorithm for identifying the PTMs in tandem mass spectra with database search. DTW is a technique that is widely used in speech recognition area. It makes a non-linear mapping of one signal to another by minimizing the distance between the two signals. In our work, for each experimental spectrum, we generate a database that contains the sequences whose parent mass values are within a certain distance from the experimental spectrum. We then compute the difference matrix between each experimental spectrum and each theoretical spectrum generated from each sequence of its database. A b-ion set and y-ion set will be generated from the difference matrix. A deterministic finite automata is then developed to determine the PTM location. Finally, DTW is used to compute the distance between the experimental spectrum and each theoretical spectrum. The results on 2657 experimental spectra with one PTM showed that the accuracy has been significantly improved while higher efficiency compared with the previous approaches.

Biography

Dr. Chunmei Liu is Associate Professor in the Department of Systems and Computer Science of Howard University. Dr. Liu received her Ph.D. in Computer Science from the University of Georgia in 2006 and then joined Howard University. When pursuing her Ph.D., she was mainly trained in Algorithms and Computational Biology focusing on non-coding RNA gene search and peptide sequencing problems. Dr. Liu received NSF CAREER award in 2009 for her research on computational proteomics.