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Identifying and locating PTMs in complex peptides or proteins based on acquired high resolution Full-Scan and MS/MS data

Until recently, most mass spectrometry biomarker discovery strategy focused on small peptide fragments ignoring the post translational landscape of larger peptides and intact proteins. Top down proteomics analyzes the intact protein and all its post translational modification in one single run. Here we describe an extension to a new top-down proteomics algorithm developed at Merck called MAR. The software runs on Linux clusters, relies only on a predefined list of 'differential' modifications (e.g., phosphorylation) and a FASTA-formatted protein database, and is not constrained to full-length proteins for identification. The added functionality to the recently published work elaborates on techniques that locate post-translational modifications within high scoring candidate polypeptide matches. These candidates are then further scored to determine the location of the modified residue. Since the publication, the software has been re-written several times and is now equipped to handle many simultaneous PTMs within a single polypeptide and determine each of their residue locations. The application of these new developments for protein id may be very useful in areas such as neuroproteomics and neurology.

Biography

Ray Fyhr has an AB degree from Colgate University and an MS degree in Computer Science from New York Institute of Technology. With over 30 years of professional experience as a software developer and business analyst, his career has traversed many industries including pharmaceutical, communications, financial, transportation, manufacturing, and operations research. In 2004, Mr. Fyhr joined Merck supporting the information technology needs of the Proteomics department. This included a customized LIMS deployment and other lab automation endeavors involving Elucidator and HPC. Of particular interest to Ray is developing software which solves complex research problems. Now he is involved with implementing new algorithms for Top-Down Proteomics and other types of biomarker analyses.

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