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Identification of short peptides in proteomic studies using database searching

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A common approach to identify the peptides in tandem mass spectrometry (MS/MS) experiments is to use database search software that compares the MS/MS spectra against theoretical spectra derived from a database of known and putative peptide sequences. These software packages use the identification of multiple peptides resulting from artificially induced cleavage for robust identification of the precursor protein. In addition, longer peptides are likely to result in more informative spectra and more unambiguous identification. This situation does not apply to the detection of individual and typically short neuropeptides that result from the natural cleavage of prohormone proteins. The performance of three open-source database search software to identify neuropeptides was studied and characterized. A collection of 7850 known and predicted rat peptides from prohormone cleavage by protein convertases was compiled. The peptide sequences were used to simulate 23550 ideal, uniform MS/MS spectra without post-translational modifications under a range of conditions including neutral mass loss, charge state and missing ions. The simulated spectra were searched across a database that included all known and predicted peptides. Across threshold P-values, Crux correctly matched all the simulated spectra to the corresponding peptides in the database meanwhile OMSSA and X!Tandem failed to correctly recognize a few spectra. Small peptides less than 10 amino acids in length were difficult to match at stringent significance levels. At a threshold P-value < 0.01, more than 64% and 75% of the 6- and 7-residue peptides were correctly identified by Crux. At a threshold P-value < 0.01, Crux, OMSSA, and X!Tandem correctly detected 98.3%, 99.9%, and 97.4% of the peptides respectively. Successful identification of short neuropeptides requires tailored detection criteria based on peptide size rather than a single global threshold.

Biography

Malik Nadeem Akhtar is a Ph. D. graduate student of Bioinformatics in the Department of Animal Sciences at the University of Illinois, Urbana-Champaign. He received his B. Sc. in Bioinformatics from the COMSATS Institute of Information Technology, Pakistan and a M. Sc. in Bioinformatics from the University of Illinois at Urbana-Champaign. His research focuses on developing algorithms and systems to accurately identify peptides in mass spectrometry studies of biomedical models.