Frank Kjeldsen, J Proteomics Bioinform 2013, 6:7
http://dx.doi.org/10.4172/0974-276X.S1.067

OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference on
Proteomics & Bioinformatics
July 15-17, 2013 Courtyard by Marriott Philadelphia Downtown, USA

Application of intensified complementary ions formed in tandem mass spectrometry to identify co-isolated peptides in complex samples

Frank Kjeldsen
University of Southern Denmark, Denmark

A critical element of mass spectrometry-based proteomics is to relate with high statistical significance experimental obtained tandem mass spectrometry (MS/MS) data to peptide sequences from a protein database. Interestingly, among all fragment ions in MS/MS spectra exists a subset of sequence specific complementary ion pairs (e.g. bn/ym-n, with m being the peptide length) of considerable high reliability. Here, we investigated the reliability of complementary ion pairs formed in CAD and CAD/ETD MS/MS and developed a reliability-based approach of intensification of these ion signals prior to database searching. Such intensification should afford higher yield of peptide identification in database searching with Mascot. In a large-scale proteomics experiment using high-resolution orbitrap MS, an increase in the number of peptide identifications was obtained relative to the original CAD MS/MS spectra when intensified CAD/ETD complementary (+18.6%) and CAD complementary pairs (+17.2%) were submitted to the Mascot search engine. This also exceeded the results obtained by deisotoping/deconvolution of CAD MS/MS spectra. Extending this approach afforded efficient extraction of sequence specific complementary ions of co-isolated peptides. For all MS/MS spectra, a matrix was constructed to calculate the sum of all combinations of possible complementary pairs corresponding to peptide monoisotopic masses present in close proximity to the isolation window of the target peptide. After this, *n+1* spectra were constructed, with n being the number of virtual spectra comprising intensified complementary ions from co-isolated peptides. All together, these approaches demonstrated an impressive gain of 42.4% more peptide identifications ($p<0.05$) compared to that of the CAD unprocessed data set.

Biography

Frank Kjeldsen (Chemistry, University of Southern Denmark (SDU), 2001: Ph.D., Biological Mass Spectrometry, SDU/Uppsala University, 2004) has been an associate professor at SDU since 2009. After graduation he completed post-doctoral studies both at Uppsala University and later at SDU. Frank has an extensive record of studying novel gas-phase ion-electron reactions and their application to biological mass spectrometry. In his current position, he is focused on mass spectral interrogation, novel chemistries in proteomics and developing methodology and theory in mass spectrometry with the goal of reaching in-depth protein and peptide characterization. He has published close to 50 papers in peer-review journals.

frank@bmb.sdu.dk