

Peptide fragmentation algorithms

Peptide identification software currently used in proteomic studies take into account little if any of the abundance information generated from tandem mass spectrometry data, thereby losing the potential to improve identification accuracy and confidence. The goal of this project is to identify peptide fragmentation patterns by bio-informatic analysis of thousands of spectra for peptides of known sequence, and the development of peptide identification software which uses as much of the spectral data as possible, with the ultimate goal of improving accuracy and confidence in proteomic investigations.

We call our algorithm SQID, which stands for SeQuence IDentification. The 28,311 spectra that were used to develop this algorithm are available to the public and will hopefully be used for the greater good of peptide fragmentation algorithm development. For more information on these spectra please see our publication - Y. Huang, J. M. Triscari, G.C. Tseng, L. Pasa-Tolic, M. S. Lipton, R.D. Smith, V. H. Wysocki "Statistical Characterization of the Charge State and Residue Dependence of Low-Energy CID Peptide Dissociation Patterns" *Anal. Chem.*, 2005, 77(18), 5800-5813 and contact tcherny@email.arizona.edu to acquire these spectra.