



The Synergies of Mass Spectrometry and Informatics

John R. Yates, III

The Scripps Research Institute

Mass spectrometry has always had a powerful synergy with computers. Computers have pushed mass spectrometry forward at key junctures in its history from data collection to instrument operation to data analysis. Proteomics was enabled by both tandem mass spectrometry and informatics to rapidly assign amino acid sequences to spectra. As instrumentation has become more powerful informatic capabilities have grown to keep pace with increases in data production and data types. Sophisticated workflows are used to process proteomic experiments that encompass search, quantitation, and statistical processing of data. As new features are added to mass spectrometers like ion mobility this provides additional capability for collecting data and information for interpreting peptides and peptide features. IP2 is a proteomic platform that creates a workflow combining GPU powered search, flexible quantitation, and statistical analysis of data.