## Poster presentation

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# **A computational and analysis tool for proteomics research** Xinnan Niu, K Jill McAfee, Dexter T Duncan, Michael Assink and Andrew J Link\*

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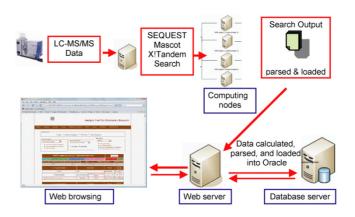
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### **Background**

Analysis Tool for Proteomics Research (ATP) is our next generation approach for processing, storing and analyzing mass spectrometry-based proteomics data base on our previously developed bioinformatics graphical comparative analysis tools (BIGCAT) software [1]. This software is being developed for the efficient management, visualization, identification, characterization and comparison of peptides and proteins from tandem mass spectrometry experiments. The basic framework of the software suite consists of a back-end relational database to store primary LC-MS/MS data and the peptide/protein identification data from various database search algorithms. The interactive front-end software applications are interfaced to the relational database for managing, visual interpreting, and analyzing the LC-MS/MS results (Figure 1). As an open source and multi-functional analysis software suite, it enables users to 1) customize source code scheme to facilitate specialized experiment aims, 2) manage and load LC-MS/ MS data and protein identification, 3) graphically display and evaluate protein identifications using various views and threshold modifications, 4) compare, merge, and run cluster results from multiple LC-MS/MS experiments, 5) search for neutral losses that are indications of modified peptides, and 6) search immunological peptide motifs. The overall goal is to increase the efficiency and simplicity of managing proteomics data while providing means of publishing and analyzing data on the web in a biologically intuitive and robust way.



#### Figure I

System Architecture of Analysis Tool for Proteomics Research (ATP). The arrow denotes the direction of the data pipeline. LC-MS/MS data are loaded into the cluster of computing nodes to perform database search. The mass spectrometry data and search results are parsed and temporally loaded into the web server, where the data is processed and stored into a relational database. Users can manage, view, analyze, and compare proteomics data by sending http request to the web server.

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