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AN EVALUATION OF OPEN SOURCE PLATFORMS FOR IDENTIFICATION AND QUANTATIVE PROTEOMICS DATA MINING

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It has been recognized that the computational and statistical analysis of MS/MS spectra poses a significant challenge for the proteomics community. Processing and analysis of proteomics data involves a complex, multistage process including raw file pre-processing, peptide assignment to MSMS experimental spectra, protein identification and further validation, and in some cases, MS-based quantitation. Public domain proteomics pipeline projects such as the Trans-Proteomic Pipeline (TPP) (Keller, et al., 2005), the OpenMS Proteomic Pipeline (TOPP) (Kohlbacher, et al., 2007), CRUX (Park, et al., 2008), and the Computational Proteomics Analysis System (CPAS) (Rauch, et al., 2006) integrate a number of open-source, cross-platform tools providing a pluggable development framework for the proteomics scientific community.

In the present work, we have evaluated a number of open-source (or freely available (academic)) packages for proteomics analysis including protein identification, validation and MS-based quantitation. Cross-platform statistical models based on False Discovery Rate or Bayesian probability for determining the confidence level of peptide and protein identification were compared in order to assess their sensitivity and specificity of such tools. MS-based quantitative analysis also suffers from the lack of cross-platform standard data formats. We have therefore evaluated a number of freely available software for iTRAQ and label-free quantative analysis. The open source nature of such packages allows us to add new functionalities to the pipeline, such as the one introduced by us in the TPP code for iTRAQ quantitation improving experimental accuracy. Finally, we provide a thorough workflow for proteomics data analysis to assist proteomics practitioners to implement open-source software pipelines.