

Label-free quantitative proteomics and a systematic analysis of *Helicobacter pylori*

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The essential role of contemporary proteomics is analysis of the entire systems, sets of proteins in the organisms or tissues rather than individual objects or events. Systems analysis that examines vital functions and development of biological organisms via different technological approaches (genomics, proteomics, transcriptomics, metabolomics) and integrates this knowledge into a system is becoming more relevant. Quantitative data set of RNA, proteins, and metabolites provides an unprecedented starting point to understand, at a systems level, the effects of perturbations on a cell [1]. To understand biology at the systems level, we should study the structure and dynamics of cellular and organismal processes, rather than the characteristics of individual parts of the cell or organism. Properties of the system as well as stability play central roles and understanding of these properties forms the future of clinical applications. However, many breakthroughs in experimental technology, advanced software and analytical methods are required before the achievements of systems biology can live up to their much-touted potential [2].

Here we conducted the search for the best methods and parameters to compare the quantitative composition of proteins between samples determined by mass-spectrometry IDA (information dependent acquisition) experiments using AB SCIEX TripleTOF 5600.

The quantification approach was based on TOPP [3] tools from OpenMS 1.10 [4] software framework. The single proteotypic peptide of highest abundance was used for protein quantification. This approach was applied to compare 8 strains of *Helicobacter pylori*, 4 strains of *Neisseria gonorrhoeae* and 2 strains of *Escherichia coli*. The proposed solution allows quantitative comparison of 80% of the identified proteins. Comparison of our results

with the results obtained using the existing commercial program Progenesis showed high similarity (Spearman correlation coefficient of 0.9).

Total running time of the proposed software solution for the quantification of the two samples was less than 1 hour, which is comparable to the time for the commercial decisions.

Particularly, the approach can be used for planning MRM (multiple reaction monitoring) experiments by searching protein of interest with the greatest difference in expression levels.

This approach was applied to 8 strains of *Helicobacter pylori*. The results of the comparative quantification were integrated with the protein-protein interaction map provided in 2001 by Jean-Christophe Rain [5].

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