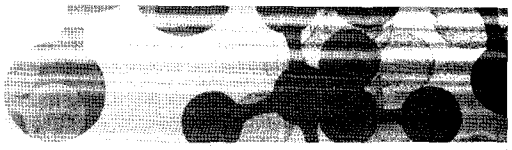

S4-3

A computational framework for systems biology approaches using LC-MS based comparative proteomics

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LC-MS based peptide profiling, in which reproducible peptide patterns are generated and compared, offers new opportunities for comparative proteomic analysis in systems biology approaches, as a fast and sensitive alternative to 2DE analyses of proteins, or LC-MS/MS based shotgun approaches. We present a computational framework for systems biology approaches using LC-MS based comparative proteomic analysis. This framework consists of 1) assessing reproducibility of LC-MS runs by visualizing and analyzing the LC-MS datasets, 2) detecting peptides in the individual datasets; 3) matching corresponding peptides across the LC-MS datasets; 4) comparing peptide abundances to select differentially expressed peptides between classes of samples; 5) identifying these selected peptides using targeted LC-MS/MS analysis; and 6) performing network/pathway analysis to understand how these differentially expressed peptides form functional modules in the networks and how these modules interact with each other to determine molecular mechanisms differentiating the two classes of samples (e.g., disease pathophysiology in healthy and diseased samples). This framework comprises two components that were originally independently developed for: *i*) LC-MS based comparative proteomics (MSAnalyzer) and *ii*) systems biology approaches using comparative proteomic data (Prequips). These two components will be demonstrated using the preliminary results of type II diabetes and drug-treated macrophage. Currently, the MSAnalyzer component, as a plugin, is being incorporated into Prequips, permitting to perform the whole framework in Prequips.