

Abstract: Biochemical information plays a key role in daily medical practice where clinical assays and a small panel of biochemicals inform a physician about health status. Biochemical knowledge is also important for all aspects of drug discovery and drug development. Information gained can be amplified significantly with an ability to measure a large array of chemicals. Technology has now matured to move biochemistry to an “omics” level from the study of one metabolite and one pathway to the comprehensive study of the “metabolome” and the metabolic network. While progress has happened in analytical chemistry and enabled creation of powerful metabolomics platforms that can yield measurements of vast number of metabolites the ability to generate biological knowledge out of this complex data has lagged behind. This is seen as one of the biggest bottlenecks in metabolomics research today. In addition large metabolomics data sets now exist where there is added genomic, transcriptomic and phenotypic data that needs to be validated, analyzed and integrated to provide biological knowledge that will further serve as important hypotheses for experimental investigations and provide models for diseases. There is a need to develop significant bioinformatics infrastructure to achieve these goals and this will form the primary focus of this application. Towards this end, we will develop an analysis pipeline that will encompass development and utilization of statistical validation and analysis of data, functional module and pathway reconstruction, and dynamic network modeling. The analysis pipeline will be biologist-friendly and will be made accessible to the metabolomics and to the larger biomedical research community. We bring pioneers in the field of bioinformatics and metabolomics who have been collaborating closely for the last several years and who bring complimentary set of skills to work closely with clinical groups to address bottlenecks in the field and create tools that can help more rapid advances in applications of metabolomics in the medical field.