Metabolome Analysis and Enzyme Information in Systems Biology

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Abstract

At the Cologne University Bioinformatics Centre (CUBIC, cubic.uni-koeln.de) we follow a concept of highly integrated experimental and theoretical (bioinformatics) research. In addition to our more "traditional" research projects on protein structure and function the main, focus in the centre is on the analysis, integration of and use of metabolome information. This includes:

· the development and application of experimental strategies for metabolome analysis,

· the statistical analysis and integration of metabolome information with genome and proteome information,

· the use of integrated metabolome and proteome data for genome annotation,

· the use of metabolome data for pathway analysis,

· the simulation of metabolic/regulatory pathways

· based on the enzyme and metabolic information system BRENDA (www.brenda.uni-koeln.de) methods for enzyme functional classification and mechanistic coding are developed.

BRENDA represents a comprehensive information system on enzyme and metabolic information, based on primary literature. The database contains data from at least 83,000 different enzymes from 9800 different organisms, classified in approximately 4,200 EC numbers. BRENDA includes biochemical and molecular information on classification and nomenclature, reaction and specificity, functional parameters, occurrence, enzyme structure, application, engineering, stability, disease, isolation, and preparation, links, and literature references. The data are extracted and evaluated from approximately 46,000 references, which are linked to PubMed as long as the reference is cited in PUBMED. The database is accessible free of charge for the academic community at http://www.brenda.uni-koeln.de

In the lecture results of metabolome analysis, the use of the data for genome annotation and the simulation of cellular behaviour will be presented as well as the use of enzyme functional data for enzyme mechanism and classification.