Structural & Functional Motifs in Metabolic Enzymes
– A new set of Functional Motifs –

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Abstract

Metabolic enzymes are responsible for the tasks of running the body at the cellular level of all types of tissues and organs. They are required for the energy production, cellular division, growth, repair and maintenance of the body in almost all kinds of organisms.

Metabolism is important for cell survival which is undertaken by specific enzymes. Healthy cells usually have normal metabolism pathways while sick cells show abnormal pathways. Understanding the function of enzymes responsible for metabolism pathways is one way to better treat metabolic related illnesses.

As it has accumulated by a vast number of research studies, 3-dimensional (3D) structure of enzymes dictates the function they do, in other words, the function of enzymes necessitate a certain 3D structure where active/binding site residues are exposed in favorable spatial environment and electro-chemical conditions that allow the carrying out of the reactions needed for their biological function.

A number of master level projects have been dedicated to carry out structural bioinformatics methods to study enzymes involved in a number of metabolic pathways including; the Citric Acid Cycle, Urea and Amino Acids Cycles, Carbohydrates and Metallic Binding proteins; the aims of which are to try and discover the underlying basis behind their biological function.

It was necessary to use spatial structures of proteins from the international database known as the Protein Data Bank or PDB which stores proteins and enzymes in complex forms with substrates or Ligands.

The study resulted in the detection, identification and description of a new group of structural elements arranged three-dimensionally in special volumes that are deemed crucially important in the specific functions of the relevant enzymes. These structural elements are called here Structural & Functional Motifs (or SFMs) together with their content of key amino acids can shed light on the underlying rules behind the biological function of proteins and be can used in a number of applications including the structure and function prediction in molecular modelling techniques and *De Novo Drug Design* of new drugs targeting metabolism related diseases.

SFMs data and the Binding Environment details have been annotated into the a number of online databases that are accessible for the URL address:
http://bioinformaticstools.org/prjs/mtbsfms/

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