Chapter 15
Enzyme Function Classification:
Reviews, Approaches, and Trends

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ABSTRACT

Enzymes are important in our life and it plays a vital role in the most biological processes in the living organisms and such as metabolic pathways. The classification of enzyme functionality from a sequence, structure data or the extracted features remains a challenging task. Traditional experiments consume more time, efforts, and cost. On the other hand, an automated classification of the enzymes saves efforts, money and time. The aim of this chapter is to cover and reviews the different approaches, which developed and conducted to classify and predict the functions of the enzyme proteins in addition to the new trends and challenges that could be considered now and in the future. The chapter addresses the main three approaches which are used in the classification the function of enzymatic proteins and illustrated the mechanism, pros, cons, and examples for each one.

INTRODUCTION

Proteins play important roles in the living organisms. They carry out a majority of the cellular processes and act as structural constituents, catalysis agents, signaling molecules and molecular machines of every biological system. It makes up a large proportion of living cells and they are important (i) as enzymes

to carry out all the metabolic reactions (biological catalysts) going on inside the cell; (ii) as structural proteins making up connective tissue, muscle, bones and the cellular division machinery; (iii) as receptors and ion channels to communicate from the outside to the inside of the cell and to allow flow of ions and small molecules across the cell membrane; (iv) as the basis of our immune system in the form of antibodies and (v) being involved in macro-molecular complexes with RNA, DNA and carbohydrate molecules (Eisenberg,2000, Gennis,2013).

Enzymes represent basic and the most important types of proteins. The enzyme or protein sequences contained in various organisms are very easy to determine, but to find experimentally the function of a protein remains a tedious and expensive task because it needs a faster and more cost-effective manner. Thus, the biologists are interested to find an automatic approach that can help them to filter among the numerous possibilities, and so with the aid of computational methods for the development of models to classify and predict the functions of various enzymes based on similarities between their sequences and/or their spatial structures (Tharwat, et al.,2015a)

The IUBMB enzyme classification system represents the first enzyme classification set by the Enzyme Commission (EC) since five decades ago to classify the enzymes and update with new enzymes which discover. IUBMB puts Enzyme Nomenclature and decided to retain the systematic names as the basis for classification for any reason, e.g. the code number alone is only useful for identification of an enzyme; systematic names stresses the type of reaction; can be formed for new enzymes by the discoverer; and the systematic names are helpful in finding recommended names that are in accordance with the general pattern.

According to above recommendations the EC develops a new scheme of enzyme classification and numbering consist of code numbers prefixed by EC which is now widely in use. The EC classification system contains four elements/numbers separated by points, the first number shows to which of the six main divisions (classes) the enzyme belongs, the second number indicates the subclass, the third number gives the sub-subclass, and finally the fourth number is the serial number of the enzyme in its sub-subclass. EC classified the enzymes based on the chemical reactions into six main classes such as (i) Oxidoreductases to this class belong all enzymes catalyzing oxidoreduction reactions, (ii) Transferases are enzymes transferring a group, e.g. a methyl group or a glycosyl group, (iii) Hydrolases these enzymes catalyze the hydrolytic cleavage of $C-O$, $C-N$, $C-C$ and some other bonds enzyme, (iv) Lyases are enzymes cleaving $C-C$, $C-O$, $C-N$, and other bonds by elimination, leaving double bonds or rings, or conversely adding groups to double bonds, (v) Isomerases these enzymes catalyze geometric or structural changes within one molecule, (vi) Ligases catalyzing the joining together of two molecules coupled with the hydrolysis of a pyrophosphate bond in ATP or a similar triphosphate (Sharif *et al.*,2015a, Tipton,1994).

The rest of the book chapter is organized as follows: Section 2 presents some of the state-of-the-art methods. Section 3 introduces a detailed explanation of enzyme function classification using sequence alignment. In this section, sequence alignment methods and the similarity score calculations are explained. Section 3 presents details about enzyme function classification using enzymes' structures. Enzyme function classification using features is introduced in Section 4. Finally, conclusions and future work are presented in Section 5.

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