

Siriwon Taewijit 2009: Enzyme Subfamily Classification and Structure Analysis
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The number of enzyme sequence grows exponentially over time. Identifying of class for a new found enzyme is usually performed by experiments in laboratory. Unfortunately, it is both time-consuming and costly. Large number of researches on enzyme classification have been carried out for decade such as (1) homology-based, this approach got high accuracy when similarity score between target and template is more than 60%. (2) subsequence-based, this approach aims to find useful portions that related to enzyme function. (3) feature-based, this approach tries to represent enzyme with the new form. Their results were able to generate good accuracy but they cannot exhibit relationships between enzyme and its structure.

In this research, we propose an enzyme subfamily classification method using residue contact and profile HMMs. Our hypothesis is based on the fact that enzyme function is directly related to its structure. First, each fragment from contact map matrix which is representative of 3D structure is extracted. Then, profile HMMs is used to build feature vector to represent each enzyme sequence. Notice that only enzymes with known PDB (11.21% of the training data) have been used to extract features. Finally, SVM was used to build a classifier. Our method yields high accuracy and provides structural description based on secondary structure contact on 3D domain. Empirical results show that our method yields 73.71% accuracy with jackknife test and the accuracy rises up to 75.87% when substitution group of amino acids is used for background knowledge. These suggest that our feature extraction from contact map and Profile HMMs are sufficiently significant for enzyme subfamily classification.

Student's signature

Thesis Advisor's signature