



生物信息学研究中心

Center of Bioinformatics

学术报告

题目 : Evolutionary matching of surface patterns
for predicting protein functions and
binding specificities

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摘要 : Predicting protein functions is a challenging task, as evolutionary relationship reflected by global sequence and structure similarities are often unreliable for function prediction. For proteins binding to similar substrates or ligands and carrying out similar functions, their binding surfaces experience similar physicochemical constraints, and hence the sets of allowed and forbidden residue substitutions are similar. We develop a method for predicting protein functions by incorporating evolutionary information specific to an individual binding region and by rapidly matching local surfaces. Our method is based on the estimation of substitution rates of amino acids. It computes a profile which characterizes protein binding activities that may involve multiple substrates or ligands. We show that our method can be used to predict enzyme functions, to identify potential substrates, and to assess binding specificity. In an objective large scale test of 100 enzyme families with 2,196 structures, our predictions are sensitive and specific: At the stringent specificity level of 99.98%, we can correctly predict enzyme functions for 80.55% of the proteins. The overall area under the Receiver Operating Characteristic curve measuring the performance of our prediction is 0.955. Our method also works well in predicting the biochemical functions of orphan proteins from structural genomics project.