





## **Center of Bioinformatics**



## 题 目: Protein Sequence Analyses for Epitope Prediction

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Abstract: Bioinformatics tools for epitope prediction assist biologists to analyze the protein sequences/structures and design peptides for antibody generation and detection of the pathogen-infected antisera. Our group has studied the functional peptides for many years. Several methodologies were developed focusing on the prediction of antigenic regions and unique peptide antigens. Linear Epitope Prediction (LEP) tool was developed for calculating the sequence antigenicity score according to the physico-chemical propensities of each amino acid. Each physico-chemical propensity score is further modified by mathematical morphology methodology. LEP is advantage to extract local peaks within the relatively low antigenicity regions, and some of them are demonstrated as real epitopes by molecular biology experiments. Except LEP, we just reported LEPS which combined physico-chemical propensities with amino acid segmental features using SVM method. LEPS enhanced large number of specificity and positive prediction value. The overall accuracy was also increased. As we know, the antibody/antigen recognition always faces the problems of binding nonspecifically. A specific antigenic peptide is crucial for generating a specific antibody. In order to pick up the unique and antigenic peptides, Reinforced Merging Unique Segment (ReMUS), an advanced version of Reinforced Merging Algorithms (RMA), was developed to analyze sequence set with high similarity, and extract the unique regions within each individual protein sequence. In the ReMUS system, the unique regions, named unique peptide motifs (UPMs), were ranked according to the antigenicity and we found that UPMs involved in molecular interaction behaviors such as antigen-antibody, protein-DNA, and ligand-receptor interactions. Our three methodologies assist molecular biologists to analyze their sequences and provide prediction for designing biological experiments.