

Prediction of Protein-Protein Binding Sites and Epitope Mapping

Computational modeling of protein-protein interactions is increasingly playing a more important role in the design and optimization of biologics. Computational methods for predicting protein-protein binding sites or epitopes have profound applications in a number of areas in the development of biologics, from understanding the mode of action to the modulation of protein properties. This work presents a novel algorithm for predicting likely antigen epitopes from protein-protein docking results using the MOE software platform. The approach generates an ensemble of poses which represent the most favorable interactions. Protein-protein residue contacts are then used to generate interaction fingerprints which serve to identify Boltzmann-weighted clusters of poses and extract consensus epitope residues. This method produces at least one predicted epitope with significant overlap to the native structure ranked in the top five clusters.