A simple and efficient method for predicting protein-protein interaction sites

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ABSTRACT. Computational methods for predicting protein-protein interaction sites based on structural data are characterized by an accuracy between 70 and 80%. Some experimental studies indicate that only a fraction of the residues, forming clusters in the center of the interaction site, are energetically important for binding. In addition, the analysis of amino acid composition has shown that residues located in the center of the interaction site can be better discriminated from the residues in other parts of the protein surface. In the present study, we implement a simple method to predict interaction site residues exploiting this fact and show that it achieves a very competitive performance compared to other methods using the same dataset and criteria for performance evaluation (success rate of 82.1%).

Key words: Interaction site prediction; Binding site prediction; Binding sites; Interaction sites; Protein structure