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Using a Domain to Predict Protein-Protein Interactions

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Abstract

The interactions between proteins are essential for many biological processes. It is vital to learn the specifics of these interactions in order to better understand the pathophysiology and therapies for different diseases. However, there are still a lot of false-positive and false-negative issues with the existing experimental methodology. A more significant prediction technique that can get over the limitations of the experimental method is computational prediction of protein-protein interaction. In this study, we suggested a brand-new computational domain-based approach for PPI prediction, and we developed an SVM model for the prediction based on the physicochemical characteristic of the domain. The results of SVM and the domain-domain score were utilized to build the protein-protein interaction prediction model.

Keywords: Posttranslational modification; Protein-protein interactions; Signal transmission; Molecular underpinnings

Introduction

Proteins are generally made up of one or more sub-molecule sections known as domains. A domain is a structural or functional module of a protein that is often composed of evolutionarily conserved elements. Differential domain association allows organisms to develop new functions. Interactions between domains can aid in the localization of a protein to a specific subcellular region, recognition of protein posttranslational modification, or participation in signal transduction. Interactions can influence enzyme activity, vigor, and substrate specificity. Many comprehensive domain studies have recently been undertaken. The PDZ domain, found in proteins such as protein tyrosine phosphatase and nitric oxide synthase, for example, plays a crucial function in regulating protein-protein interactions, protein targets, and protein complex formations. The PB1 domain is found in a variety of signaling proteins engaged in several signaling pathways, including the mitogen-activated protein kinase and cellular polarity pathways [1].

Water-protein interactions are crucial in influencing protein organization at the water interface. Water-protein interactions aid in the maintenance of the flexible conformation conditions essential for multifunctional protein recognition mechanisms. The experimental water properties measured in protein systems in solution can be used to investigate the intimate link between the protein surface and hydration water

Domain-based prediction has opened up a new window into the study of protein-protein interactions. PPIs serve an important role in biological processes such as immune response, signal transmission, and disease incidence and progression. There are two ways for predicting protein-protein interactions: experimental and computational. The first research approaches include yeast two-hybrid tandem affinity purification co-immunoprecipitation and other strategies for finding protein-protein interactions. However, high- and low-throughput experimental approaches have manpower and material limits, and experimental results frequently exhibit high false positives and false negatives.

Proteins containing the PB1 domain have been linked to the development of cancers such as breast cancer and lung cancer. More and more evidence suggests that domain anomalies can contribute to a variety of diseases. As a result, it has significant practical implications for domain-based medication design and disease therapy in clinical research, such as arteriosclerosis and cancer. Domain-based research may aid in understanding the molecular underpinnings of human diseases, developing appropriate disease models, and developing diagnostic tools. Because it is widely assumed that protein interactions are mediated by specific domain interactions, the domain-based technique has gained popularity in recent years [2, 3].

Currently, domain-based approaches' features only include domain co-occurrence connections or the proportion of an important domain. The domain information is not completely taken into account. Domain interactions are important for understanding biomolecule interactions because they provide a global picture of the protein-protein interaction network. To efficiently use domain information, we suggested a new domain-based technique for predicting protein-protein interactions [4].

Materials and Methods

Positive protein-protein interaction data were gathered from interacting adhesome protein-protein interactions. It is available at The Adhesome: A Focal Adhesion Network's website. The negative PPI data was obtained using Xiao-Yong et al.'s noninteraction dataset, in which no protein pair has sequence identity. Pan's dataset was widely used in research of protein-protein interactions.

To extract the domain of its protein, we used the protein database stated above as our source database. The Pram database was used to gather protein domains and sequence information for these domains. The corresponding domain-domain pairs were created. Meanwhile, domain pairs that interact and do not interact were chosen from the Intercoms and 3did databases. The Interim database had a set of DDI confidence scores with a cutoff of 1.5 for false-positive prediction and no false-positive prediction [5].

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Our strategy made use of the physicochemical properties of domain pairs. The domain and associated sequencing information were obtained from the Pram database. The physicochemical property of the domain can be derived using the web tools ProtParam and Procom based on the domain's sequence information.ProtParam is capable of calculating a variety of physicochemical characteristics for a given protein [6].

We performed a correlation analysis on these features to eliminate the interference of correlation variables. Finally, 10 significant physicochemical property traits were identified. They were amino acid counts, theoretical pI, and total number of negatively and positively charged residues, total number of atoms, Ext. coefficient 1, instability index, aliphatic index, grand average of hydropathicity, and domain location.

The fivefold cross-validation method divides the data into five equal halves at random. In turn, one portion serves as a testing set, while the other four serve as a training test. It efficiently prevents the overfitting issue. Simultaneously, our results have been counted at least five times till they are generally consistent.

The initial slope approximation and subsequent three-parameter exponential regression analysis of the longitudinal recovery curves were used to obtain the selective spin-lattice relaxation rates. The greatest possible experimental error in relaxation rate measurements.

Sigma Chemical Co. supplied human albumin. All of the solutions were made with D2O that had a low deuterium concentration [7, 8].

Discussion

This part is divided into four sections: the first is the intermediate result of domain-domain interaction prediction, the second is protein prediction, the third is a comparison of other methods, and the fourth is our model's limitations.

The SVM prediction model is generated using the domain's physicochemical property. Five times cross validation was performed to check the dependability of the results, assess the robustness of our method, and restrict the impact of data independence. Five SVM calculations were carried out.

The predicted structure of the protein revealed the sequence identity; the binding pocket was adjacent to two Cu2+ ions. Since the crystallographic structure of human protein has not been determined, it is unknown which residues in the protein structure are glycosylated. A prior study found that human protein was heavily glycosylated, and that it is linked to the proper folding to create the active enzyme.

A protein-protein prediction model was built using the Interdom database's domain-domain interaction score and DDI predicted label results. To lessen the numerical disparity between domain-domain scores.

The average accuracy of prediction. The F1 and MCC indicators can be used to assess the classifier's overall performance. The F1 and MCC average values. These findings demonstrate that the physicochemical qualities of a domain provide efficient feature information for domain-domain interaction; with the interacting domain-domain we predicted outperforming the total theoretical domain pairs in a protein pair [9-13].

Conclusions

The authors developed a new domain-based technique for predicting protein-protein interactions in this publication. The protein interaction-predicting model was built using the domain's physicochemical properties and interaction score. The projected result, a good performance, implies that our strategy is generally successful. The domain's physicochemical properties are important features for PPI prediction. Our future study will include applying our approach to huge datasets and discovering more effective feature information for predicting PPI. Furthermore, our approaches can be utilised to predict novel PPIs, and the results may have some relevance for dealing with relevant bioinformatics problems.

Conflicts of Interest

None

Acknowledgment

None

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