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Compressed Images for Affinity Prediction (CIFAP): A novel machine learning methodology on protein-ligand interactions

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Known protein-ligand interactions are worth to analyze in order to design safe and efficient drugs and to help drug discovery and development. Recently, intelligent techniques have been found useful in drug design. It is possible to gather information from known interactions and to predict specific properties of the unknown interactions with the help of bioinformatics and machine learning. The aim of this study is to propose a novel computational methodology, which is called Compressed Images for Affinity Prediction, CIFAP, to predict binding affinities of structurally related protein-ligand complexes. The CIFAP method is based on a protein-ligand model from which computational affinity information is obtained by utilizing 2D electrostatic potential images determined for the binding site of protein-ligand complexes. The study has two phases, namely, data modeling and prediction. After each ligand is docked to the protein, the binding site is isolated from the complex as the binding pocket of the protein with its ligand. The isolated 3D structure is located into an electrostatic potential grid box which is then compressed through three orthogonal directions into three 2D images for each protein-ligand complex. Sequential forward selection technique is applied in order to obtain patterns from the images and to avoid redundant features in prediction. The quality of the CIFAP method is tested using Support Vector Regression (SVR) and Adaptive Neuro-Fuzzy Inference System (ANFIS) which are highly promising prediction methods in drug design. The computational algorithm presented here is proposed to have a great potential in pharmacophore-based drug design.

Biography

Erdem Buyukbingol received his Ph.D. from Ankara University and postdoctoral studies from Case Western Reserve University, OH. He is a Professor of Medicinal Chemistry.

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