Evaluation and Ranking of Protein Docking Models by 3D Convolutional Neural Networks

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Protein-protein interactions, which occur at protein-protein interfaces, are essential for biological activities. Understanding the mechanics of protein binding and predicting new interactions requires identifying protein-protein interface areas. It's crucial to be able to determine protein-protein interactions quickly and accurately. Protein-protein complex structure is required to extract a protein interface. Because finding a single protein complex structure experimentally requires time and effort, computational docking technologies that can offer thousands of alternative complex structures, called decoys, in a short amount of time are promising. The ability to distinguish near-native decoys from thousands of proposed decoys is a hurdle using computational approaches. DeepInterface, a three-dimensional convolutional neural network-based decoys scoring and ranking system, was enhanced in this work. We analyzed different convolutional neural network architectures and explored the hyperparameter space to discover the highest performing DeepInterface model that resembled VGG16. We created positive datasets from the Protein Data Bank complexes and negative datasets from the PPI4DOCK and DOCKGROUND docking databases' erroneous decoys. We demonstrated that the model that was proposed originally can accurately distinguish positive interfaces, such as those recorded in the PDB, from erroneous ones using the CAPRI criterion, with the accuracy of 81%.