

Scoring geometries of protein-protein complexes

Florian Krull¹, Myong-Ho Chae², Ernst-Walter Knapp¹

¹Institute of Chemistry and Biochemistry, Freie Universität Berlin

²Department of Biology, University of Science, Unjong-District, Pyongyang

Interactions between proteins are known to play a central role in many biological processes. However, it is often easier to obtain structural information of the individual proteins instead of the whole protein complex. Hence, there is need for theoretical procedures that can predict protein complex structures given the structures of the individual proteins. Many algorithms try to solve this problem. The currently used methods typically generate many possible protein complex geometries (decoys) considering shape complementarity only. To discriminate near-native geometries from false positives these decoys are ranked by a scoring function. To train learning-based scoring functions we generate decoys primarily for the purpose of training. We demonstrate the impact of carefully chosen sets of training decoys on the performance of two different learning-based scoring methods.