

Computational Method for Modeling Protein Assembly with More Than Two Protein Subunits

Predicts multi-protein complex assembly more accurately than existing methods.

Researchers at Purdue University have developed a model for predicting protein-protein docking. Software previously developed for predicting protein-protein interactions includes CombDock. The Purdue software, called Multi-LZerD, uses a more rigorous physics-based approach to model the interactions. The model also uses the 3D Zernike descriptor (3DZD) to allow a level of soft-docking to influence the docking prediction. The Multi-LZerD software is an improvement on the researchers' previous work; it allows more than two protein-protein interaction predictions among many proteins. For final selection of the most-favorable docking, a small translation and rotation is applied to each of the most-favorable protein-protein pairs .

Technology Validation: Multi-LZerD outperformed CombDock for 8 out of 10 tested unbound docking cases with more than two subunits and had slightly worse performance for the 10 bound docking cases with more than two subunits.

Advantages:

â€¢ Better performance than CombDock for unbound docking cases

Applications:

â€¢ Predicting protein-protein interactions for more than two subunits

Related Publication: Multi-LZerD: multiple protein docking for asymmetric complexes. Esquivel-Rodr  guez J, Yang YD, Kihara D. Proteins. 2012 Jul;80(7):1818-33. doi: 10.1002/prot.24079.

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