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Computational Method for Modeling Protein Pairwise Assembly

LZerD is an accurate, automatic computational model for predicting protein-protein interactions and docking structures, enabling advancements in drug design and elucidating biological signaling pathways.

Researchers at Purdue University have developed a model for predicting protein-protein interactions called LZerD. Protein-protein interactions mediate many biological processes, and deciphering the protein interactome can help elucidate signaling pathways and drive drug design. Researchers have developed various methods for protein interactome predictions governed by different interaction parameters. The Purdue researchers' method searches the scientific literature for protein-protein interface information and predicts the most likely docking structures based on ranking of statistical scoring performance. The top scoring structures are then relaxed by a molecular dynamics simulation to resolve atom clashes and improve side-chain conformations. In rounds 38-46 of the Critical Assessment of Prediction of Interactions (CAPRI), a protein interactome prediction competition, the Purdue researchers' model was a top performer in the server group. Evaluation of the server group relies on the performance of the automatic model itself, with no post-prediction manual refinement by research teams. The researchers have also expanded their work with the development of Multi-LZerD technology, software that can predict the interactome of more than two protein subunits.

Related Publication: Performance and enhancement of the LZerD protein assembly pipeline in CAPRI 38-46. Proteins. 2020 Aug;88(8):948-961. DOI: 10.1002/prot.25850.

Technology Validation: In rounds 38-45 of the CAPRI competition, the researchers' model predicted the structure of the protein-protein interface at an acceptable or higher level in 15/22 cases (68.2%).

Advantages:

- Automatic

Technology ID
2021-KIHA-69434

Category
Biotechnology & Life Sciences/Bioinformatics & Computational Biology
Artificial Intelligence & Machine Learning/AI Model Optimization & Acceleration Tools
Pharmaceuticals/Computational & Software Tools

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- Accurate -- award-winning accuracy in CAPRI

- Able to consider experimental constraints

Applications:

- Protein interactome predictions

TRL: 4

Intellectual Property:

Copyright, N/A, United States

Keywords: Protein-protein interaction prediction, LZerD, Multi-LZerD, protein assembly pipeline, CAPRI, docking structures, molecular dynamics simulation, protein interactome, multimeric protein docking, genetic algorithm