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Computational Method for Modeling Disordered Protein Assembly

First reliable computational tool for modeling disordered protein–protein interactions.

Purdue University researchers have developed a computational docking method for modeling the structure of disordered protein-protein interactions (PPIs) dubbed IDP-LZerD. Protein-protein docking is extensively utilized in the biotechnology, pharmaceutical, and biomedical industries to model the three-dimensional structure of protein complexes. Current docking methods are predominantly optimized to model the complex formation of ordered protein partners, whose three-dimensional structure is assumed to remain constant upon binding. However, intrinsically disordered proteins (IDPs) do not adopt a single three-dimensional structure, and current docking strategies do not reliably model IDP-involved PPIs. IDPs serve critical roles in the regulation of PPIs across various biological pathways, but current tools cannot accurately model these interactions. IDP-LZerD is a first-of-its-kind method that utilizes biophysical principles to reliably model the conformation of the disordered protein in PPIs involving long IDPs up to 69 amino acids. IDP-LZerD performs than existing methods in producing docking models with correct bound conformations. Notably, IDP-LZerD was able to correctly model longer IDPs when compared to two other methods. These results highlight the utility of IDP-LZerD for structural modeling of disordered protein interactions.

Technology ID

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Category

Biotechnology & Life Sciences/Bioinformatics & Computational Biology

Artificial Intelligence & Machine Learning/AI Model Optimization & Acceleration Tools

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Advantages

-Accurate modeling of protein-protein interactions with long intrinsically disordered proteins (IDPs)

-Novel computational method that follows the known biophysical mechanisms of IDPs

Applications

-Computational Protein Modeling

-Modeling 3D structures of disordered ligand-receptor pairs

-Drug discovery

-Biotechnology

Technology Validation:

-Produced docking models with correct bound conformations with better performance than existing methods

-Correctly modeled longer IDPs when compared to two other methods

Related Publications :

Modeling disordered protein interactions from biophysical principles

PLoS Computational Biology

DOI: 10.1371/journal.pcbi.1005485

IDP-LZerD: Software for Modeling Disordered Protein Interactions

Methods in Molecular Biology

DOI: 10.1007/978-1-0716-0708-4_13

TRL: Biotechnology

Intellectual Property:

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