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Computational Method for Drug Screening using Molecular Surface Information

PL-PatchSurfer2.0 is a computational software tool that predicts drug candidate binding characteristics for target proteins, enhancing the efficiency of the drug discovery and design process.

Researchers at Purdue University have developed a software called PL-PatchSurfer2.0 that predicts binding characteristics of drug candidates or other ligands for target proteins. PL-PatchSurfer2.0 considers four surface characteristics of both the drug and protein and accounts for the different shapes that the ligand can take to predict how the ligand binds to the protein. PL-PatchSurfer2.0 takes a unique approach to modeling the surface of the protein and ligand, making it a useful part of the drug discovery toolkit. Recently, PL-PatchSurfer2.0 demonstrated its effectiveness in the D3R Grand Challenge 4 competition, performing competitively at ranking the affinity of a series of compounds for each of two target proteins, beta-secretase 1 and cathepsin S.

Technology Validation: PL-PatchSurfer2.0 performed competitively among a field of other computational tools at ranking the affinity of a series of compounds for each of two target proteins, beta-secretase 1 and cathepsin S.

Advantages

-Performs well with proteins that undergo structural change upon binding

-Compatible with computationally modelled target protein structures

Applications

-Drug discovery

-Drug design

-Computational biology

Related Publications

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Category
Biotechnology & Life Sciences/Bioinformatics & Computational Biology
Artificial Intelligence & Machine Learning/AI Model Optimization & Acceleration Tools
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Predicting binding poses and affinity ranking in D3R Grand Challenge using PL-PatchSurfer2.0.

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Intellectual Property:

Keywords: PL-PatchSurfer2.0, drug discovery, drug design, computational biology, ligand binding prediction, target proteins, protein-ligand interaction, affinity ranking, molecular modeling, beta-secretase 1, cathepsin S