PURDUE INNOVATES | Office of Technology Commercialization

PL-PatchSurfer: Molecular Surface-based Method for Exploring Protein-ligand Interactions

PatchSurfer is an alignment-free, surface-based pocket comparison program that accelerates the design of new ligands for a wide array of drug targets by quickly identifying similar binding pockets.

Interactions with small ligand molecules are essential aspects of proteins and there is an urgent need for computational methods for function prediction. A major drawback of current approaches is the dependency on the chemical features present in the known actives.

Researchers at Purdue University have addressed this major drawback by developing an alignment free, surface-based, pocket comparison program called PatchSurfer. PatchSurfer represents a binding pocket as a combination of segmented surface patches, with each patch characterized by its geometrical shape, the electrostatic potential, the hydrophobicity, and the concaveness. The device searches a database of known pockets and finds similar ones based on the surface patch similarity. Because each surface patch characterizes geometrical and physicochemical properties of a protein pocket and ligand on a continuous surface, the surface representation is less sensitive to subtle changes on the pocket and ligand conformation. This aspect helps to quickly allow a better understanding of protein-ligand interactions, and ultimately, can help to enhance the design of new ligands for a wide array of drug targets.

Advantages:

-Less sensitive to subtle changes on the pocket/ligand conformation

-Faster search speed

-New ligands for a wide array of drug targets

Potential Applications:

-Ligand design

Technology ID

2015-KIHA-67111

Category

Biotechnology & Life Sciences/Bioinformatics & Computational Biology

Pharmaceuticals/Computational & Software Tools

Pharmaceuticals/Research Tools & Assays

Authors

Bingjie Hu

Daisuke Kihara

Woong-Hee Shin

Xiaolei Zhu

Further information

Joe Kasper

JRKasper@prf.org

Nathan Smith

nesmith@prf.org

View online

-Virtual screening

-Pharmaceuticals

-Drug targets

TRL: 5

Intellectual Property:

Keywords: PatchSurfer, protein-ligand interactions, computational methods, function prediction, alignment free, surface-based, pocket comparison, binding pocket, ligand design, virtual screening