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SSnet: A Deep Learning Approach for Protein-Ligand Interaction Prediction

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Abstract

Computational prediction of Protein-Ligand Interaction (PLI) is an important step in the modern drug discovery pipeline as it mitigates the cost, time, and resources required to screen novel therapeutics. Deep Neural Networks (DNN) have recently shown excellent performance in PLI prediction. However, the performance is highly dependent on protein and ligand features utilized for the DNN model. Moreover, in current models, the deciphering of how protein features determine the underlying principles that govern PLI is not trivial. In this work, we developed a DNN framework named SSnet that utilizes secondary structure information of proteins extracted as the curvature and torsion of the protein backbone to predict PLI. We demonstrate the performance of SSnet by comparing against a variety of currently popular machine and non-machine learning models using various metrics. We visualize the intermediate layers of SSnet to show a potential latent space for proteins, in particular to extract structural elements in a protein that the model finds influential for ligand binding, which is one of the key features of SSnet. We observed in our study that SSnet learns information about locations in a protein where a ligand can bind including binding sites, allosteric sites and cryptic sites, regardless of the conformation used. We further observed that SSnet is not biased to any specific molecular interaction and extracts the protein fold information critical for PLI prediction. Our work forms an important gateway to the general exploration of secondary structure based deep learning, which is not just confined to protein-ligand interactions, and as such will have a large impact on protein research.

Biography

Niraj Verma is an artificial intelligence enthusiast and had applied its application to various sectors of science, majorly focused on chemistry and biology. Niraj Verma has more than a decade of experience in python. Niraj Verma started his professional journey as a polymer chemist from the Indian Institute of Technology (top technical universities in India) and his keen interest in computers landed him a job as a software engineer in a website development company ScheduleOnce. Following the passion for chemistry, Niraj Verma joined the Computational and Theoretical Chemistry Group (CATCO) as a research scholar working towards holy-grail problems such as protein structure prediction, novel drug discovery, protein-drug interactions, non-covalent bonds and their strength in protein and water systems, etc. Apart from academia, Niraj Verma enjoys practicing Tae-kwon-do (black belt), play guitar, and on some rare occasions visit the gym.

Publications

- Deep Learning-Based Ligand Design Using Shared Latent Implicit Fingerprints from Collaborative Filtering
- Halogen Bonding Involving I2 and d8 Transition-Metal Pincer Complexes
- Systematic Detection and Characterization of Hydrogen Bonding in Proteins via Local Vibrational Modes
- Predicting Potential SARS-COV-2 Drugs-In Depth Drug Database Screening Using Deep Neural Network Framework SSnet, Classical Virtual Screening and Docking
- Deep Learning-based Ligand Design using Shared Latent Implicit Fingerprints from Collaborative Filtering

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