THE USE OF AI AND ADVANCED COMPUTER SYSTEMS TO DEVELOP DRUGS AGAINST NEW EMERGING THREATS

Utilizing Geometric Deep Learning To Enhance The Accuracy Of Preclinical Identification Of Drug Candidates

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Drug discovery is a resource-intensive multi-year endeavor. In particular, the optimization of the drug across multiple properties is a particularly labor and time intensive bottleneck. Predicting the chemical composition of a new preclinical drug is particularly challenging because the combination of properties typically relies on the chemical composition of the protein pocket of interest. Recent breakthroughs in protein structure prediction like AlphaFold, have vastly expanded access to structural data, highlighting the urgent need for efficient methods to optimize diverse targets across various properties. Despite the abundance of protein structural data, we don't have a way to identify the 3D structures and molecular compositions of ligands that populate those pockets more efficiently.

At Stanford, we pioneered a method utilizing geometric deep learning to directly generate new ligands within protein pockets. Our software optimizes ligands across numerous properties. MachinaMinds, a company we founded, is dedicated to commercializing this technology to streamline drug discovery, reducing the time and resources required to develop new drugs.

ACS Central Science,
Geometric Deep Learning for Structure-Based Ligand Design