Machine Learning Aided Rational Drug Discovery and Design

We *accelerated* the drug discovery process.

Client:
Confidential

Sectors:
Medicine
Pharmacology

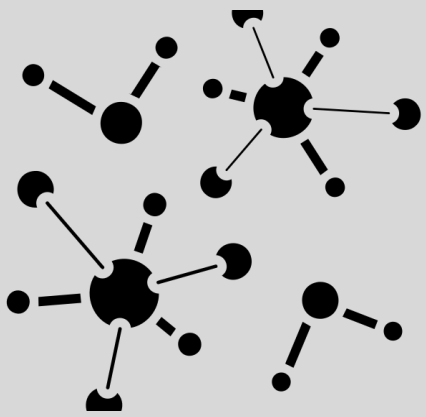
Technologies:
High Performance Computing (HPC)
Molecular Dynamics Simulations
Machine Learning
AlphaFold
Ligand Binding Models
Chemical Synthesis ML Models
Stochastic & Probabilistic Modeling
Parallel Computing
Python
TensorFlow
PyTorch

Resources:
https://clutch.co/profile/dreamers#reviews

Challenge: The drug discovery process is expensive and time-consuming, requiring extensive in vitro and in vivo testing to identify viable compounds. Our client needed a highly efficient digital drug discovery pipeline capable of rapidly generating, screening, and optimizing drug candidates while minimizing computational costs and maintaining accuracy. Additionally, the solution needed to integrate the latest advancements in machine learning and computational chemistry to enhance ligand binding predictions and synthetic pathway analysis.

Solution: We developed a comprehensive high-performance computing (HPC) pipeline for rational drug design, leveraging fragment libraries to generate massive pools of drug candidates. These were screened based on lipophilicity and metabolic stability (e.g., CYP450 cleavage likelihood), followed by large-scale parallelized simulations to minimize energy and RMSD. Our approach balanced stochastic and probabilistic modeling to optimize resource efficiency while maintaining high accuracy. We incorporated AlphaFold's architecture to train ligand binding models and built an end-to-end ML-driven chemical synthesis platform that suggests optimal synthetic pathways based on thousands of chemical heuristics.

Result: Our solution enabled the client to generate highly targeted receptor agonists for in silico assays, significantly reducing the need for costly in vitro and in vivo testing. By leveraging state-of-the-art machine learning and high-performance computing, we accelerated the drug discovery process, improving efficiency and precision while reducing costs.



> **"The problem of designing drugs is essentially the problem of approximating the solution to Schrödinger's equation for energy in 3D space. It's not a simple task, and they delivered a lot of value to our team of experts."**