Computer Science Laboratory of the École Polytechnique (LIX), UMR 7161
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DeepEnzyme

#MedTech #ProteinStructure #DeepLearning

THE PROBLEM ADDRESSED

Our AI targets in-silico drug design, developing algorithms and software to assess molecule efficiency and discover new active compounds.

The project relies on a cooperation between two laboratories from Ecole Polytechnique, combining their expertise in deep learning, structural bio-informatics, and biochemistry.

This cross-functional approach aims to enhance the accuracy of screening processes, reducing experimental costs and shortening development time. By identifying weak molecular interactions early, it increases the likelihood of hit identification, ultimately improving the overall efficiency of drug discovery and advancing the development of successful treatments.

TECHNOLOGY

The team is developing a hybrid in-silico approach for large-scale drug prediction.

Their AI consists of:

- A multimodal, physics-inspired deep learning approach predicting quantitative protein-ligand interactions (PLI) by incorporating a novel AI-based solvation model. This approach leverages recent developments in Large Language Models (LLMs) and Graph Machine Learning (GML) by analyzing protein structures as both amino acid sequences and geometric graphs.
- Fitting of state-of-the-art diffusion and geometric graph neural network models for molecules and proteins, addressing modern challenges in drug discovery.
- The unique strength of our AI model lies in its training on a dataset generated from physics-based simulations, which is significantly larger than available experimental data. This makes our AI more universal, robust, and accurate.

COMPETITIVE ADVANTAGES

- A unique database built from public data, enriched with experimental results from École Polytechnique. We leverage in-house expertise on proteins dependent on vitamin B9, key targets for anti-microbial and anti-cancer therapies.
- A novel state-of-the-art deep learning approach incorporating protein, molecule and solvent information.

APPLICATIONS

- Identification of new uses for existing drugs (repurposing)
- Discovery of novel molecules (hit discovery)
- Development of potent anti-microbial drugs
- Innovation in oncological treatments

DEVELOPMENT STATUS

- TRL3-4: the findings our Deep Learning model are being consolidated and begin to be experimentally validated

INVENTORS & CONTACTS

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PUBLICATIONS

- Qabel, Aymen, et al. "*Structure-Aware Antibiotic Resistance Classification Using Graph Neural Networks*." NeurIPS AI4Science (2022).
- Aleksandrov A and Myllykallio H. "*Advances and challenges in drug design against tuberculosis: application of in silico approaches.*" Expert Opinion on Drug Discovery 14.1 (2019): 35-46.

LOOKING FOR

- Collaborations on new molecules with industrial partners
- Access to empirical databases (active and inactive molecules related to the cellular targets)