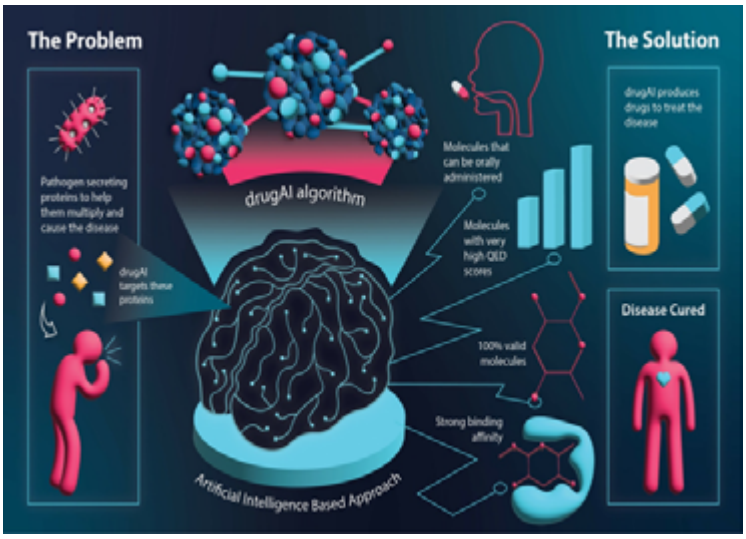
CHAPMAN UNIVERSITY | Office of Research

De Novo Drug Design Using Transformer-Based Machine Translation and Reinforcement Learning of an Adaptive Monte Carlo Tree Search

Chapman Case #2024-004

Market Need

The global pharmaceutical industry is constantly seeking innovative solutions to streamline drug development pipelines and expedite the identification of promising drug candidates. Traditional methods such as high-throughput screening, although effective, are often resource-intensive and time-consuming, hindering the rapid advancement of life-saving therapies. Pharmaceutical companies require an innovative platform that can rapidly generate novel, valid, and drug-like small molecules with strong binding affinities to specific targets, enabling accelerated drug discovery pipelines, reduced development costs, and faster time-to-market. In the current age of artificial intelligence adoption, the companies that can leverage the growing power of generative AI would gain significant competitive advantages in their drug discovery efforts.



Chapman Solution

Chapman University has developed a novel artificial intelligence platform, named drugAI, that integrates transformer-based machine learning and reinforcement learning techniques to generate novel, valid, and drug-like small molecule structures with strong binding affinities to specific protein targets. The platform offers unique benefits that would make it an ideal solution for pharmaceutical companies to accelerate their drug discovery pipelines:

- 100% validity rate, significantly higher quantitative estimates of drug-likeness (up to 42% improvement)
- Adherence to physicochemical constraints like Lipinski's Rule of Five
- Comparable and/or higher binding affinity from the docked small molecules to target protein vs conventional virtual screening method(s)
- Able to optimize multiple objectives simultaneously

Applications

- De novo design of potential drug candidates for a wide range of diseases, including cancer, cardiovascular diseases, and neurodegenerative disorders.
- Exploration of novel chemical spaces for the identification of unique scaffolds and chemotypes.
- Multi-target drug design for complex diseases requiring polypharmacological approaches.

Key Publication

"De Novo Drug Design Using Transformer-Based Machine Translation and Reinforcement Learning of an Adaptive Monte Carlo Tree Search", MDPI, January 2024.

Stage of Development

- Demonstrated proof of concept that outperformed other models.
- Available for further research collaborations.

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