A Novel Computational Approach to Drug Discovery Through Drug Repositioning

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Current processes of drug discovery are too long, expensive, and ineffective. Companies undergo years of research and development without the certainty of obtaining conclusive results. Drug repositioning is emerging as an effective and less capital-intensive way to repurpose pre-existing drugs to treat new conditions. Using data from DrugBank about drug-disease and drug-drug interactions, two different computational models were developed. The first takes input from a user about a new disease and provides drugs that may be suitable candidates; this model uncovers novel relationships by mapping pre-existing drugs to the new condition. The second model was built using an artificial intelligence GNN (graphical neural network). It takes in drug-drug relationship information in order to map out interactions. The model is trained to predict different relationships such as drug compatibility and FDA approval. Together, these models can facilitate and replace many steps of the drug discovery cycle. The results are promising: the first model effectively searches through data and returns the most appropriate drugs for a novel symptom, and the GNN maps out and predicts drug relationships up to an accuracy of 84%. This has tremendous real-world applicability. One of the main issues that can be addressed is the opioid problem - medical professionals overprescribe opioids for patients, continuing addictions. Finding alternative treatment options would be instrumental in curbing this problem. Further, these models can be used by medical professionals to find the effective treatment options for chronic conditions which do not have definite treatments.

Awards Won:
National Anti-Vivisection Society: Third Award of $2,500