

AI-Powered Drug Discovery: Integrating Chemistry, Biology, And Data Science

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Abstract:

“The integration of chemistry, biology and data science into Artificial Intelligence (AI) is rapidly re-defining the drug discovery landscape, to enable accelerated and improved identification of potential therapeutics. In this research we learn to apply four machine learning and two deep learning algorithms namely: Random Forest (RF), Support Vector Machine (SVM), Convolutional Neural Network (CNN), and Graph Neural Network (GNN) for molecular property prediction and virtual screening. These models were trained and evaluated on a comprehensive bioactive compounds dataset. Compound-target interactions are predicted with better performance of CNN and GNN models achieving accuracy of 91.4% and 93.2% respectively. On contrast, RF and SVM results for accuracy was 87.6 % and 85.1 %, respectively. Precisen, recall and F1 scores are used for comparing and GNN achieves an F1 score of 0.92. The second, the study also touts AI’s efficiency in cutting down drug discovery timelines and computational costs. The proposed AI driven solution is effective and novel, and is enhanced with the results of comparative analysis with existing literature. These findings highlight the enormous opportunities of AI in reshaping contemporary pharmacology and delivering high quality, low cost, and rapid scale-up in early stages drug development.”

Keywords: Drug Discovery, Artificial Intelligence, Deep Learning, Molecular Prediction, Virtual Screening.

I. INTRODUCTION

Drug discovery, the traditional process that typically spans 5–8 years and requires significant financial investment, is characterized by high attrition rates and inefficiencies. Traditionally, the techniques often resort into trial and error, in vitro, and animal model experimentation, all of which prolong the timing and increase cost. In the last decade, the usage of Artificial Intelligence (AI) in drug discovery has been very much talked about as a method to resolve these coupled challenges [2]. AI powered tools are being used to revolutionize the way researchers go about identifying potential drug candidates, predict the potency of