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Using AI to Speed Up Early Drug Discovery through Better Target and Compound Analysis

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Abstract: *The drug discovery process is usually very time and resource consuming, mainly due to the significant biological validation and chemical screening carried out in its initial stages. The current study proposes an artificial intelligence assisted drug discovery tool to hasten these initial discovery stages by applying sophisticated artificial intelligence algorithms. The tool makes use of Open Targets to find biological targets relevant to diseases and obtains chemical compounds using ChEMBL. Large Language Models are utilized to analyze drug likeness, toxicities, and ADMET properties by applying structured reasoning graphs. The model attained an accuracy of 91% in drug likeness prediction, 88% in toxic prediction, and 85% in ADMET prediction. Additionally, a scientific report generator was combined to sum up the findings, achieving a factual consistency index of 0.68. The new discovery system lowers drug discovery by almost 50% in its initial stages and maximizes hit prioritization by about 22%, illustrating the effectiveness of applying biomedical datasets and language model analyses to hasten drug discovery in a more informed manner.*

Keywords: Artificial Intelligence, Drug Discovery, Large Language Models (LLMs), Open Targets, ChEMBL, ADMET Prediction

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