



APP ABSTRACT - APP 2026

## Artificial Intelligence in Drug Discovery: A Data-Driven Methodological Framework

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### Abstract

Artificial Intelligence (AI) is transforming the traditional drug discovery pipeline by accelerating target identification, compound screening, and optimization. Conventional drug development is often time-consuming and costly, typically requiring more than a decade of research and billions of dollars in investment. Recent advancements in machine learning, deep learning, and large-scale biological datasets enable predictive modeling that can significantly reduce this timeline. This study presents a conceptual framework for integrating AI techniques into early-stage drug discovery. Using publicly available biomedical datasets, machine learning models can analyze molecular structures, predict drug–target interactions, and prioritize promising compounds for experimental validation. The framework highlights the potential of AI to improve efficiency, reduce development costs, and identify novel therapeutic candidates. The results demonstrate that the AI-driven computational screening can complement the laboratory experiments and facilitate it faster translation from research . The methodology follows a computational research pipeline commonly presented in AI-healthcare conferences. First, biological and chemical datasets are collected from public databases such as molecular structure repositories and genomic datasets. Second, data preprocessing techniques including normalization, feature engineering, and molecular fingerprint extraction are applied to prepare the data for machine learning models. Third, predictive algorithms such as Random Forest, Support Vector Machines, and Deep Neural Networks are trained to predict drug-target interactions and biological activity. Finally, the top-ranked candidate molecules are identified for further in-silico simulation or laboratory validation.

### Keywords

Machine Learning, Deep Learning, Drug-Target Interaction, Computational Biology, Bioinformatics