Abstract

According to the FDA, drugs are substances intended to diagnose, cure, alleviate, treat, or prevent diseases. Despite rigorous clinical trials, adverse drug reactions (ADRs) rank among the top 10 leading causes of death in some countries. Conventional drug research methods involving in vivo and in vitro testing require significant time and resources, prompting the need for efficient computational approaches. This study introduces a novel integration of the Artificial Bee Colony (ABC) algorithm with ensemble models for feature selection and ADR prediction, specifically focusing on reproductive system and breast disorders. By leveraging data from the Side Effect Resource (SIDER), three ensemble techniques were evaluated: Random Forest, AdaBoost, and XGBoost. The ABC algorithm optimized feature sets, and hyperparameter tuning further enhanced model performance. Random Forest demonstrated superior performance, achieving an accuracy of 0.6311 and an F1-Score of 0.6770. These results highlight the potential of the proposed ABC-ensemble framework in advancing early-stage ADR detection, offering a computationally efficient and scalable solution to improve drug safety assessment in drug discovery.

Keywords: Artificial Bee Colony, Ensemble Learning, Feature Selection, Random Forest, Drug Side Effects, Reproductive System Disorders, Hyperparameter Tuning