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A Novel Framework for Drug Approval Prediction using Chemical Structure with Knowledge Distillation

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In the pharmaceutical field, productivity in new drug development is decreasing noticeably. This decline is largely attributed to the increasing costs associated with research and development and a simultaneous decrease in the rate of new drug discoveries. As a response to these challenges, pharmaceutical companies are actively pursuing strategies to not only predict the ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) properties but also to assess the probability of success of drug candidates through computational techniques.

Previous studies used clinical trial results to predict the likelihood of success of drug candidates. However, clinical trials are costly, limited, and difficult-to-grasp information. These methods are unlikely to be of great help in the pre-clinical phase of drug discovery.

In our study, we proposed a novel framework to directly predict the approval of drug candidates in pre-clinical stage. Our framework evaluation indicated high and robust predictive capabilities compared to other machine learning models when using solely chemical structure information to predict the approval of drug candidates. Furthermore, we validated the feasibility of predicting approvals for drug candidates by leveraging data from FDA-approved drugs in 2023.

Our study provides a broadly applicable strategy to identify promising drug candidates at the pre-clinical stage. We hope that our study will provide valuable support to the research community, contributing to the evaluation and enhancement of the drug development process.