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Modeling Optimal Lipophilicity and Drug Performance in Ligand-Receptor Interactions: A Machine Learning Approach to Drug Discovery

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Abstract : The drug discovery process currently requires numerous years of clinical testing as well as money just for a single drug to earn FDA approval. For drugs that even make it this far in the process, there is a very slim chance of receiving FDA approval, resulting in detrimental hurdles to drug accessibility. To minimize these inefficiencies, numerous studies have implemented computational methods, although few computational investigations have focused on a crucial feature of drugs: lipophilicity. Lipophilicity is a physical attribute of a compound that measures its solubility in lipids and is a determinant of drug efficacy. This project leverages Artificial Intelligence to predict the impact of a drug's lipophilicity on its performance by accounting for factors such as binding affinity and toxicity. The model predicted lipophilicity and binding affinity in the validation set with very high R^2 scores of 0.921 and 0.788, respectively, while also being applicable to a variety of target receptors. The results expressed a strong positive correlation between lipophilicity and both binding affinity and toxicity. The model helps in both drug development and discovery, providing every pharmaceutical company with recommended lipophilicity levels for drug candidates as well as a rapid assessment of early-stage drugs prior to any testing, eliminating significant amounts of time and resources currently restricting drug accessibility.

Keywords : drug discovery, lipophilicity, ligand-receptor interactions, machine learning, drug development
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