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Abstract

Machine Learning Strategies for Drug Discovery in AML: Focus on RUNX1 Bioactivity †

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Acute myeloid leukemia (AML) is an aggressive blood cancer where immature stem cells in the bone marrow multiply rapidly, disrupting blood cell production and leading to infections, anemia, and bleeding. This devastating disease claims around 85,000 lives annually and is projected to double by 2040, highlighting its critical importance for research and improved treatment strategies. The RUNX1 transcription factor, a critical gene for hematopoiesis, is highly prevalent in AML and linked to poor patient outcomes. Mutations disrupt RUNX1's function, essentially acting as a "bad switch" that promotes aggressive leukemia growth and significantly reduces survival chances. Targeting this master regulator holds promise for developing novel therapies to improve patient outcomes in AML.

In the current study, we utilized a computational drug discovery approach, involving bioactivity data retrieval for Human RUNX1 "CHEMBL2093862" from the CHEMBL database, where RUNX1 is the target protein. We performed chemical space analysis using Lipinski descriptors to identify whether the compounds have the properties of ideal drugs or not. We calculated molecular descriptors, specifically PubChem fingerprints, to identify the unique structure of the compounds. We applied machine learning algorithms, like Random Forest, Linear Regression, Decision Tree, and XGBoost, to create a model with the ability to classify whether the compounds are active or inactive. This study uses a user-friendly bioactivity prediction app using Streamlit so that researchers can check for the bioactivity and potency of drugs in real time for the targeting of RUNX1 in AML. This study introduces a comprehensive plan for drug development targeting RUNX1, offering potential interventions for AML mediated by RUNX1.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/proceedings2024100012/s1, Conference Poster: Machine Learning Strategies for Drug Discovery in AML: Focus on RUNX1 Bioactivity.

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