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Name of Scholar: Tanya Liyaqat
Name of Supervisor: Prof. Tanvir Ahmad
Name of the Department: Computer Engineering
Topic of Research: Applications of Machine Learning in Drug Discovery

Findings

1) Enhanced Prediction Models: The thesis aims to improve the drug discovery process by developing advanced prediction models for drug-target interaction (DTI), drug-target binding affinity (DTBA), and molecular properties like mutagenicity.

2) Effective Techniques: Research shows that DTI and DTBA predictions are significantly enhanced through effective data balancing, careful modality selection, and the application of machine learning (ML) and deep learning (DL) algorithms.

3) Stacked Ensemble Model: Integrating various ML classifiers into a stacked ensemble model greatly improves the accuracy of mutagenicity predictions, leveraging multiple modalities for comprehensive analysis.

4) Multi-Modal Approach: By incorporating sub-structural, physicochemical, geometric, and topological features, the multi-modal approach captures a broader range of molecular characteristics, resulting in more robust and accurate predictive models.

5) Impact on Drug Discovery: The findings such as the analysis of structural alerts facilitate the early identification of mutagenic compounds, potentially reducing development costs and preventing unsafe candidates' progression. This research offers innovative methodologies for safer and more efficient drug development processes.