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DEEP LEARNING-BASED MOLECULAR SCREENING OF A-SYNUCLEIN

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Abstract

Drug discovery is a complex process that involves identifying molecules that can interact with specific molecular targets in the body to treat diseases. Parkinson's Disease (PD) is the second most affected in neurodegenerative disorder and there is no cure but treatment focusses on managing the symptoms. Targeting α-synuclein is high-priority in PD research as it is aimed to develop disease-modifying treatment rather than symptom management. However, the complexity lies in the intrinsically disordered nature of α-synuclein and the severe class imbalance present in the available bioactivity datasets. In early-stage virtual screening, preserving potential active molecules is more critical than achieving high classification accuracy. In this research deep-learning based virtual screening model is proposed to prioritize small-molecule modulators of α-synuclein with high recall and early enrichment.

The model employs deep fusion architecture which integrates molecular fingerprint and physicochemical descriptors to capture non-linear chemical patterns relevant to bioactivity. Rather than depending on fixed decision threshold, compounds are ranked using predicted probabilities and evaluated using enrichment-oriented metrices suitable for large-scale screening. The model is trained using weighted loss function to address extreme class imbalance and is optimized specifically for ranking performance. Experimental evaluation demonstrates strong enrichment with an enrichment ratio of 36.96 at the top 500 ranked compounds and consistent improvement in identifying active compounds when screening depth is increased. The result indicates that the proposed deep learning approach effectively reduces chemical search space while retaining a substantial fraction of active compounds. Finally, this research work highlights the importance of recall-based deep learning models for virtual screening and demonstrates their suitability for scalable α-synuclein-targeted drug discovery in Parkinson's disease.

Keywords: Deep Learning, Virtual Screening, α-Synuclein, Small-Molecules