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Drug Repurposing Through Molecular Docking: Identifying Novel Tyrosine Kinase Inhibitors

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Tyrosine kinases play a pivotal role in cellular signalling pathways that regulate cell proliferation, differentiation, and survival. Aberrant tyrosine kinase activity is implicated in the progression and metastasis of various cancers, making these enzymes critical targets for anticancer therapy. Although several tyrosine kinase inhibitors (TKIs) have been approved by the FDA, drug resistance and adverse effects remain clinical challenges. This study aims to apply in-silico drug repurposing techniques to identify FDA-approved drugs with potential inhibitory activity against tyrosine kinases involved in cancer. Utilising molecular docking, a curated library of FDA-approved compounds was screened against the ATP-binding site of target tyrosine kinase proteins, including well-characterised cancer-related isoforms. The docking protocol was performed using PyRx and AutoDock Vina, evaluating binding affinities and interaction profiles to prioritise candidate drugs. Top-ranking compounds were analysed for their binding modes and key interactions with critical tyrosine kinase residues. The repurposing approach facilitates the rapid identification of existing drugs that may be repositioned as tyrosine kinase inhibitors, bypassing early-stage drug development hurdles. This computational screening provides insights into potential multitarget agents with improved efficacy and safety profiles. The results lay the groundwork for further experimental validation and clinical evaluation of identified candidates, which could accelerate the availability of novel therapeutic options against tyrosine kinase-driven cancers. This study underscores the utility of silico molecular docking as a cost-effective, time-efficient approach in anticancer drug discovery and repositioning strategies.

Keywords: Cancer therapy, Drug repurposing, In-silico screening, Molecular docking, Tyrosine kinase inhibitors (TKIs)

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