TETRA-C: Accelerating Cancer Therapy Through AI-Optimized Telomerase Inhibition, Enzymatic Targeting, and the Suppression of Metastasis

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Cancer is a complex disease affecting millions globally, encompassing various types such as breast, pancreatic and brain cancers, each requiring tailored treatment. A crucial enzyme in many cancers is telomerase, which is present in 80-90% of cancer cells. Telomerase promotes cell longevity and inhibits programmed cell death (apoptosis). Traditional drug discovery is often costly and time-consuming, typically taking 10-15 years, while cancer cells can mutate rapidly. This study aims to streamline drug discovery by utilizing the AI model to predict and optimize new ligands targeting telomerase. To achieve this, pre-existing ligands and telomerase structures were sourced from the Protein Data Bank (PDB) and pre-processed in UCSF ChimeraX. Molecular docking was conducted using PyRx (Autodock Vina) to obtain binding affinity and RMSD values. The AI model was trained on known inhibitors and binding affinities in google colab, employing DeepChem, GPR and RDKit. This led to the generation of novel ligands with pre-defined molecular properties. Statistical analysis indicated that most of the AI-generated ligands were significantly distinct ($p < 0.05$) from the original inhibitors. The AI was able to analyze and extract valuable information regarding the inhibitors. Notably, BIBR1532, an original ligand used for baseline comparison, showed superior binding affinity. However, an AI generated ligand with similar structure and slight modifications exhibited a lower RMSD value than BIBR1532. These findings demonstrate the potential of AI in drug discovery, emphasizing the need for further optimization to develop drug-like molecules, paving the way for personalized cancer treatments and advancements in precision medicine.

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