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Title of thesis: Virtual Screening for High-Throughput Structure-Based Selection of the Best Anticancer Molecular Candidates Using Selenium and Zinc Oxide Nanoparticles in Common Cancers

Summary:

Cancer, as the second leading cause of mortality worldwide, remains one of the most significant challenges in the field of healthcare. Treating this disease is particularly challenging due to the similarity between cancerous and healthy cells, necessitating precise and targeted approaches that selectively eliminate cancer cells while minimizing damage to healthy tissues. In this context, nanotechnology provides advanced tools to develop novel targeted therapies. However, the success of such therapies depends on the accurate identification of molecular targets and optimized compounds. Molecular screening, as a rapid, precise, and cost-effective method, plays a critical role in this process. This approach not only accelerates the design of new drugs but also reduces research and development costs, opening new horizons for producing effective and affordable cancer therapies.

In this regard, the use of nanoparticles, particularly zinc oxide (ZnONPs) and selenium nanoparticles (SeNPs), has gained attention as an innovative approach to combat cancer. This study investigates the interactions of these nanoparticles with key proteins involved in cancer progression, including fibroblast growth factor receptor (FGFR1), cyclin-dependent kinase (CDK2), and cytokines CCR7 and CXCR4.

To analyze these interactions, bioinformatics methods such as molecular docking and molecular dynamics simulations were employed. The three-dimensional structures of the proteins and nanoparticles were prepared and optimized, followed by simulation and detailed interaction analysis using Autodock Vina and GROMACS software. Key parameters such as binding energy, root mean square deviation (RMSD) and root mean square fluctuation (RMSF) were assessed.

Molecular docking results revealed that zinc oxide nanoparticles exhibit lower binding energy with the target proteins compared to selenium nanoparticles, indicating their higher affinity for interaction. Specifically, ZnONPs showed stronger interactions with FGFR1 and CDK2 proteins. Furthermore, molecular dynamics simulations confirmed that ZnONPs demonstrated greater stability in their interactions with proteins

This study concludes that zinc oxide nanoparticles, due to their higher stability and stronger interactions with target proteins, are more suitable candidates for targeted cancer therapies. Their utilization can enhance the efficacy of anticancer treatments while reducing the side effects associated with conventional therapeutic approaches. The integration of nanotechnology and molecular screening represents a promising strategy for the development of novel and efficient methods to combat cancer.

Keywords: Nanoparticles, Targeted Cancer Therapy, Molecular Docking, Molecular Dynamics, Virtual Screening