Computational Assessment of Apigenin as a Prospective Protein-Based Therapeutic Targeting Mucin-1

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Mucin-1 MUC1 is a high molecular weight glycoprotein that can overexpress, causing various cancers and playing a significant role in tumor progression and metastasis. Developing targeted therapies against MUC1 presents a promising strategy for cancer treatment. Apigenin is a naturally occurring flavonoid abundant in fruits and vegetables and has been shown to produce anticancer effects. This research paper presents a computational assessment of apigenin as a prospective protein-based therapeutic targeting MUC1. This study utilized computational tools to identify apigenin as a prospective drug and analyze the binding affinity, binding modes, and stability of the apigenin-MUC1 complex. The ADMET analysis and lead optimization of apigenin were also evaluated to study the safety and improve the efficiency of the apigenin on MUC1. Molecular docking results reveal favorable binding interactions between apigenin and MUC1, suggesting a potential inhibitory effect on MUC1-related processes. The drug property, drug-likeness, ADMET analysis, and lead optimization results showed that apigenin is safe for human consumption, has all the qualities and descriptors of a drug, and can be improved in future studies. In conclusion, this computational assessment offers insights into the interaction between apigenin and MUC1, suggesting apigenin's potential as a protein-based therapeutic agent targeting MUC1-associated cancers. The lead optimization showed ten potential binding sites and five new modifications to apigenin. This study contributes to the computational drug discovery field and outlines future experimental research on apigenin-based therapies for cancer treatment. Keywords: mucin-1, apigenin, molecular docking, ADMET analysis, lead optimization, computational drug discovery