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Designed Purine Molecules and in-silico Evaluation of Aurora Kinase Inhibition in Breast Cancer

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Abstract : Aurora kinase enzyme, a protein on overexpression, leads to metastasis and is extremely important for women's health in terms of prevention or treatment. While creating a targeted technique, the aim of the work is to design purine molecules that inhibit in aurora kinase enzyme and helps to suppress breast cancer. Purine molecules attached to an amino acid in DNA block protein synthesis or halt the replication and metastasis caused by the aurora kinase enzyme. Various protein related to the overexpression of aurora protein was docked with purine molecule using Biovia Drug Discovery, the perpetual software. Various parameters like X-ray crystallographic structure, presence of ligand, Ramachandran plot, resolution, etc., were taken into consideration for selecting the target protein. A higher negative binding scored molecule has been taken for simulation studies. According to the available research and computational analyses, purine compounds may be powerful enough to demonstrate a greater affinity for the aurora target. Despite being clinically effective now, purines were originally meant to fight breast cancer by inhibiting the aurora kinase enzyme. In in-silico studies, it is observed that purine compounds have a moderate to high potency compared to other molecules, and our research into the literature revealed that purine molecules have a lower risk of side effects. The research involves the design, synthesis, and identification of active purine molecules against breast cancer. Purines are structurally similar to the normal metabolites of adenine and guanine; hence interfere/compete with protein synthesis and suppress the abnormal proliferation of cells/tissues. As a result, purine target metastasis cells and stop the growth of kinase; purine derivatives bind with DNA and aurora protein which may stop the growth of protein or inhibits replication and stop metastasis of overexpressed aurora kinase enzyme.

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