In Silico Study of Phytochemicals from Tecomella undulata Targeting CDK2 in prostate cancer

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Abstract

Prostate cancer remains a significant health concern, encouraging the search for effective and safer therapeutic options. CDK2, a key regulator of the cell cycle, is known to contribute to unchecked cellular growth when dysregulated, making it an important target in cancer research. In this work, we carried out an in-silico investigation of phytochemicals from *Tecomella undulata* to evaluate their potential to inhibit CDK2 (PDB ID: 2A4L). Among the screened compounds, Diazoprogesterone showed the most promising interaction with the CDK2 active site, exhibiting better binding behaviour than the standard inhibitor, Roscovitine. The ligand engaged with essential catalytic residues, suggesting its ability to interfere with CDK2's functional activity. Overall, the findings point toward Diazoprogesterone from *Tecomella undulata* as a compelling natural candidate for further exploration in CDK2-targeted prostate cancer therapy.

Keywords: *Tecomella undulata*, CDK2, Diazoprogesterone, Molecular Docking, Prostate Cancer