Proteins Linked to Colon Cancer: Ornithine Decarboxylase and Cox-2

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Introduction

Colon cancer exists as a major international health concern since it causes millions of new cases together with related deaths throughout the year. Colorectal cancer manifests an uncontrolled growth of cells combined with genetic alterations that produces destructive tumor growth and results frequently in metastasis. The research examined how proteins influence colon cancer initiation through a detailed study of Ornithine Decarboxylase (ODC) and Cyclooxygenase-2 (COX-2). The key molecular and cellular agents for colorectal cancer (CRC) development are Ornithine Decarboxylase (ODC) and Cyclooxygenase-2 (COX-2), as they contribute to tumor progression and therapeutic resistance.

Materials and methods/Methodology.

Energy reduction was performed using PyRx prior to docking by downloading the 3D structure of the compounds and the reference medication from the PubChem online database. Molecular docking analysis was conducted with BCP and VIT-D using some colon cancer-related proteins, including ornithine decarboxylase and COX-2 using AutoDockVina and the results were compared with the standard, 5-fluorouracil. The 2D and 3D visualisations of the interactions were generated using the Biovia Discovery Studio visualizer v21.1.0.20298.2.11.

Results and discussion

Betacaryophellene molecule showed modest activity against the ornithine decarboxylase and COX-2.

Vitamin D showed the best binding affinity (-8.1 and -7.1 kcal/mol) with strong hydrogen bonding. However, its binding energy was more than that of betacaryophellene(-6.5 and -6.7 kcal/mol) and 5-fluorouracil (−5.6 and -5.6 kcal/mol,) respectively.

Ornithine decarboxylase (ODC; EC 4.1.1.17) possesses transformative and carcinogenic and increased levels of ODC and polyamines are associated with cellular proliferation and carcinogenesis.

Molecular docking is a structure-based drug discovery method that reveals electrostatic properties including charge distribution and binding site design (the presence of clefts, cavities, and sub-pockets) to help prescreen compounds as possible medicines. The results were compared after a selection of chemicals were assessed for their binding affinities against the cyclooxygenase-2 enzyme (COX-2) (PDB ID 5IKR). The stability of the best-docked configuration is determined by the ligand-critical amino acid bonds that are formed. The hydrogen bond interaction is crucial for bioactivity after hydrophobic contacts.

Conclusions

Betacaryophellene demonstrated a more favorable safety profile, while 5-FU exhibited established toxicity concerns.While 5-FU remains a cornerstone of colorectal cancer treatment, the study suggests that betacaryophellene or exploring optimized Vitamin D formulations could enhance therapeutic efficacy.

Keywords: Colon Cancer, Ornithine Decarboxylase and Cyclooxygenase-2