

IDENTIFICATION OF NEW ANTAGONIST AGAINST LUNG CANCER THOROUGH MOLECULAR DOCKING AND PHARMACOPHORE MODELLING APPROACH

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ABSTRACT

Lung Cancer is one of the most common Cancers in the world. It is a leading cause of cancer death in men and women in the United States. Cigarette Smoking causes most lung cancer. The more cigarettes you smoke per day and the earlier you started smoking, the greater your risk of lung cancer. High levels of pollution, radiation and asbestos exposure may also increase risk

HDAC2 gene product belongs to the Histone deacetylase family. Histone deacetylases act via the formation of large multiprotein complexes and are responsible for the deacetylation of lysine residues at the N-Terminal regions of core histone (H2A, H2B, H3 & H4). This Protein forms transcriptional repressor complexes by associating with many different proteins, a mammalian Zinc-finger transcriptional factor. Thus, it plays an important role in transcriptional regulation, cell cycle progression and development events. Alternative splicing results in multiple transcript variants.

Analysis of docking results reveals that all predicted molecules binding well in the active site of HDAC2 (PDBID: 5IWG) all ligand active site residues, the molecule ZINC000010120338 showed strong binding energy and pharmacophore generation was performed with six features and by auto search 178 Unique compounds hits were obtained. These Zinc database compounds may act as potential anti-cancer agents to treat lung Cancer.

KEY WORDS: Lung Cancer, Molecular Docking, Pharmacophore Modelling.

INTRODUCTION:

Cancer is caused by changes to the DNA within the cells by accumulated damage to genes. Cancer is caused by certain changes to genes, in which uncontrolled growth and divisions of cells occur. Cancer can start almost anywhere in the human body, which is made up of trillions of cells. Normally human cells grow & divide to form new cells as the body needs them. Cancerous tumors are malignant, which means they can spread into or invade nearby tissues. In addition, as these tumors grow, some cancer cells can break off and travel to distant places in the body through the blood or the lymph system and form new tumors.