عنوان مقاله:

bioinformatics investigation of pharmaceuticalligands based on histone deacetylase cocrystal tofacilitate the transcription of tumor suppressor genes

محل انتشار:

اولین کنگره بین المللی ژنومیک سرطان (سال: 1402)

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خلاصه مقاله:

Introduction: Cancer is one of the non-infectious and malignantdiseases, which is known as a health problem and affectsthe health of the society.In addition to genetic changes, epigenetic changes are also effectivein the occurrence of cancer. One of the epigenetic mechanismsis the structural changes of histone proteins that lead tothe expression or lack of expression of a series of genes in thecell.Histone deacetylases are a group of enzymes whose job is toremove the acetyl group from an amino acid in a histone molecule,allowing it to bind more tightly to DNA. This is veryimportant because DNA is wrapped around histones and DNAexpression by The process of acetylation or deacetylation isregulated.In recent years, the role of cancer suppressor genes in the processof cell cycle regulation has been identified. If the cell cyclegoes out of normal, these tumor suppressor genes are activatedand lead the cell to apoptosis. Failure to express these genes cancause uncontrolled and cancerous cell growth. Lack of tumorsuppressor genes causes uncontrollable division of cancer cells.Deacetylation of histones by the enzyme histone deacetylase isone of the reasons for the non-expression of these tumor suppressorgenes.Considering that the resistance to anticancer drugs is increasingand also the side effects caused by the use of these drugsare many, the discovery and synthesis of new anticancer compoundswith less side effects and higher potency seems necessary.Methods: Considering the importance of inhibiting histonedeacetylase enzyme in cancer treatment, in this study, the inhibitoryeffect and the binding method of cocrystal-based pharmaceuticalligands to the active site of histone deacetylase enzyme as well as the detailed investigation and identificationof the binding mechanism of the designed compounds to theactive site of the enzyme by molecular docking method. Theresults are analyzed.Autodock۴ software is used for docking. For this purpose, atfirst, the appropriate crystallographic structure of the histonedeacetylase enzyme containing the central catalytic part is selectedand downloaded from the protein database website athttp://www.rcsb.org/PDB. Then docking is done in ۶ steps.In this study, in order to investigate the binding of the existingcompounds to the active site of the enzyme, drawing the chemicalstructure of the compounds, energy optimization and finalanalyzes were done with DS Visualizer, Hyperchem, Chem-Draw software respectively.Results: ... In the insilico section, all the studied compounds wereable to occupy the active site of the enzyme, and among all of

کلمات کلیدی:
Bioinformatics-pharmaceutical ligands-cocrystalhistonedeacetylase-tumor suppressor genes