

عنوان مقاله:

Bioinformatics approach for potential inhibitory of pyrogallol in ovarian cancer by Cdc25A targeting

محل انتشار:

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خلاصه مقاله:

Introduction: Pyrogallol, one of the natural polyphenols, was known to have anti-inflammatory and antitumor effects in some cancers. However, the underlying antitumor mechanisms of pyrogallol, still remain unclear so far. Cell division cycle 25 A (Cdc25A), is one of the most vital cell cycle regulators, and positively controls the functions of CDKs that lead to cell cycle progression. Overexpression of Cdc25A promotes tumorigenesis, and is observed in ovarian cancer. Therefore, the present study aimed to determine the potential therapeutic effect of pyrogallol for Cdc25A inhibition. **Methods:** Pyrogallol structure was drawn in the HyperChem software. Cdc25A protein structure was retrieved from the RCSB PDB database. For molecular docking and preparation of ligand and target protein, Autodock 4.2 was used. Cdc25A protein structure docking studies were performed with this software. Nonpolar hydrogen atoms were assembled and fixed in ligand. **Result:** According to the molecular docking studies, pyrogallol showed high binding energies with Cdc25A protein, with maximum values of -34.22 kJ/mol. pyrogallol mostly interacts with H, R, K, S, G, I amino acids. **Conclusion:** This evaluation concludes that pyrogallol may be used as an anticancer drug for ovarian cancer as it can suppress Cdc25A proteins and may stop the cell proliferation in cancers. Pyrogallol is recommended as an effective, safe, and commercial drug to inhibit tumor progression in patients with ovarian cancer.

کلمات کلیدی:

Key words: Pyrogallol; Cdc25A; ovarian cancer; in silico

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