

عنوان مقاله:

Bioinformatic studies of the effect of Curcumin glucuronide in the plants of the Curcuma longa species on DNA gyrase inhibition as antimicrobial agent

محل انتشار:

سومین کنگره بین المللی و چهارمین همایش ملی زیست فناوری گیاهان دارویی و قارچهای کوهی (مجازی) (سال: 1400)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

Background & Objective: DNA gyrase is an essential bacterial enzyme that catalyzes the ATP-dependent negative super-coiling of double-stranded closed-circular DNA. DNA gyrase has long been known as an attractive target for antibacterial drugs. Curcumin is a polyphenol, found in the spice turmeric, that has promising anticancer and antimicrobial properties. The aim of this research is the bioinformatical study of DNA gyrase inhibition by a Curcumin derivative. **Material & Methods:** In order to investigate the mode of interaction of the compound with DNA gyrase active site, the chemical structure of Curcumin glucuronide was designed using ChemDraw program, then transferred into Hyperchem software for energy minimization. Docking study was performed by AutoDock ۴.۲ program and the resulting docking poses were analyzed in AutoDockTools, DS Visualizer ۳.۵ and Ligplot software. **Results:** Curcumin glucuronide was able to occupy the active site of the enzyme. In fact, this compound indicated favorable interactions with the key amino acid residues at active site of DNA gyrase. Docking results for this compound are in accordance with those of co-crystallized ligand. The Gly۷۷, Glu۵۰, Thr۱۶۵, Val۱ of DNA gyrase were the sites for hydrogen bonding interactions with this compound. **Conclusion:** Finally, in respect to high effectiveness and docking results, we can conclude that the Curcumin glucuronide may be regarded as antimicrobial agent.

کلمات کلیدی:

In Silico Approach, Docking, Curcumin glucuronide, DNA gyrase

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