عنوان مقاله:

Computational molecular docking simulation study of Kojic acid glucoside as antibacterial agents

محل انتشار:

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خلاصه مقاله:

Kojic acid is a fungal metabolic product produced by a few species of Aspergillus, especially by A. oryzae, which has the Japanese common name koji. This compound is an inhibitor of growth of bacteria and multiplication of viruses. In this study, kojic acid derivative, Kojic acid glucoside, was evaluated as DNA gyrase activity inhibitors. DNA gyrase has long been known as an attractive target for antibacterial drugs. In order to investigate the mode of interaction of the compound with DNA gyrase active site, the chemical structures of kojic acid glucoside wase 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. Binding model and the best docked pose of this compound showed Kojic acid glucoside formed a hydrogen bond with Asp۷۳, Asn۴۶, Glu۵۰, Thr۱۶۵, Val۷۱, Arg۱۳۶ of DNA gyrase in active site. The insilico molecular docking study results showed that, Kojic acid glucoside have minimum binding energy and good affinity toward the .active pocket, thus, this may be considered as inhibitor of DNA gyrase

کلمات کلیدی:

Enzyme inhibition, Molecular Docking, Kojic acid glucoside, DNA Gyrase