

عنوان مقاله:

Study of effect the Quercetin on Pre apoptosis factors BAD, BAK and BIM by simulation and molecular dynamic

محل انتشار:

دوازدهمین کنگره بین المللی سرطان پستان (سال: 1394)

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خلاصه مقاله:

Introduction & Aim: Quercetin is an effective compound which is found in many herbal drugs. Quercetin antioxidant properties against cancerous tumors and apoptosis induction have been demonstrated. This study is aimed to investigate the molecular dynamics of quercetin with regards to activating the preapoptotic factors such as Bim, Bak, and Bad using simulation software. **Methods:** In this study, the thermodynamic properties of flavonoid molecule of quercetin on three important factors in apoptotic pathway such as Bim, Bak, and Bad were investigated. After the threedimensional structure of these molecules was obtained from NCBI and simulation was done by Gromacssoftware, docking stages were performed by AutoDock software and then the molecular dynamics of the complexes were investigated by Gromacs software **Results:** The number of hydrogen bonds between quercetin and Bad was higher than Bak and Bim, which causes Bad to have lower energy than Bak and Bim. Mean root-mean-square deviation at 10 ns of simulation increased for Bad and Bak and decreased for Bim in quercetin presence. Root-mean-square fluctuation investigations indicated that Bim had the highest flexibility in quercetin presence compared to free state. **Conclusion:** Computational studies indicated that quercetin could have a greater effect on Bad compared to Bak and Bim. However it is necessary to investigate the effect mechanism of quercetin on these three pre-apoptotic factors in experimental studies

کلمات کلیدی:

Apoptosis, Quercetin, Molecular Dynamic

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