

عنوان مقاله:

Study of cinnamaldehyde and eugenol binding to catalase using molecular docking approach

محل انتشار:

بیستمین کنگره ملی و هشتمین کنگره بین‌المللی زیست‌شناسی ایران (سال: 1397)

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خلاصه مقاله:

Catalase enzyme is the main regulator of hydrogen peroxide metabolism that degrades hydrogen peroxide and protects cells from oxidative damages. Catalase activity changes have been observed in some diseases such as diabetes, Alzheimer s disease, and cancer. Studies have shown that inhibition of this enzyme activity can help to treat Alzheimer s and eliminate cancer cells. Cinnamon is a well-known and commonly used spice in the food industry. Cinnamon has several beneficial health effects such as anti-tumor, anti-diabetes and anti-Alzheimer s activities. Cinnamaldehyde and eugenol are the major components of cinnamon and cinnamaldehyde allocate a high percentage of cinnamon essential oil. According to the therapeutic effect of cinnamon on some catalase enzyme associated diseases, the interaction of cinnamaldehyde and eugenol as the main bioactive compounds of cinnamon with catalase studied in this research. Crystal structure of catalase was obtained from RCSB and molecular structure of cinnamaldehyde and eugenol were downloaded from zinc database. AutoDock tools, VMD and Ligplot used to determine the best binding site of catalase enzyme for cinnamaldehyde and eugenol and also for data analysis. The result elucidated that hydrophobic interactions and hydrogen bonds play the main role in the binding of these ligands to catalase. Among amino acid residues involved in the interaction, Tyr357 and His74 play important role in catalysis reaction too. Therefore, the binding of these ligands to catalase enzyme probably change its catalytic activity. The binding energy of eugenol was more than cinnamaldehyde, so eugenol stronger interaction with catalase rather than .and decreased catalase activity

کلمات کلیدی:

Catalase, Molecular docking, Cinnamaldehyde, Eugenol

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