

عنوان مقاله:

Bovine Serum Albumin Interaction with Glycyrrhizin Studied by UV-Vis Spectroscopy and Molecular Docking

محل انتشار:

هفتمین کنفرانس بین المللی توسعه فناوری در مهندسی شیمی (سال: 1402)

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خلاصه مقاله:

In this research, the interaction of glycyrrhizin (GL) with bovine serum albumin (BSA) has been investigated by UV-Visible spectroscopy and molecular docking simulation. The UV-visible spectroscopic method and molecular modeling were performed to determine the binding constant and the binding structure of the GL-BSA complex, respectively. The results of UV-visible spectroscopy showed that GL bonded to BSA with a binding constant of $K_{GL-BSA} = 49.4 (9090) \times 10^4 \text{ Lmol}^{-1}$. The results of molecular docking revealed a minimized affinity value for the first pose of GL-BSA, which was $-1192. \text{ kcalmol}^{-1}$, and four amino acids (Tyr¹⁵⁶, Thr¹⁸³, Lys¹⁸⁴, and Ala²⁰) exhibited high affinity with GL. The GL-BSA complex primarily forms based on hydrogen bonds.

کلمات کلیدی:

Binding constant, Docking, UV-Visible, Bovine serum albumin, Glycyrrhizin

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