عنوان مقاله:

Comparative studies on the interaction between glycerol polyol with bovine trypsin: spectroscopic and theoretical approaches

محل انتشار:

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

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

The aim of the present investigation was to study how polyols could affect the structure, stability, and the activity of the protease. Different spectroscopic methods, kinetics, and molecular dynamics (MD) studies were carried out to study the effect of glycerol on the activity and structure of trypsin in 50 mM Tris–HCl buffer.It was demonstrated that polyol quenched the intrinsic fluorescence of trypsin by the static quenching process. The calculated thermodynamic parameters (ΔH°<0, ΔS°<0) showed that the acting forces of complex formation between trypsin and polyol were hydrogen bonds and van der Waals forces with an overall favorable Gibbs free energy change (ΔG°<0). The increase in the absorption of trypsin in the presence of glycerol was as a result of the formation of the glycerol-trypsin complex. In addition, the kinetic studies revealed that this polyol enhances enzyme activity of trypsin, in a concentration-dependent manner. Also, molecular docking, as well as thermodynamic parameters, indicated that hydrogen bonds and van der Waals forces play important role in stabilization of trypsin- polyol complexes. Molecular docking results showed the presence of one binding site on the surface of trypsin with a negative value for the Gibbs free energy (ΔG˚) of the binding of glycerol to trypsin. Near-UV and Far-UV circular dichroism studies also demonstrated the transfer of Trp, Phe, and Tyr residues to a more flexible environment

کلمات کلیدی:

Bovine trypsin, Polyol, Enzyme activity, Intrinsic fluorescence, Molecular docking