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Solvent effects on host-guest residence time and kinetics: further insights from metadynamics simulation of Toussaintine-A unbiding from chitosan nanoparticle

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Solvent effects on host-guest residence time and kinetics: further insights from metadynamics simulation of Toussaintine-A unbiding from chitosan nanoparticle

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Abstract

Solvents play an important role in host-guest intermolecular interactions. The kinetics and residence time of Toussaintine-A (TouA) unbinding from chitosan was investigated by means of well-tempered metadynamics and thermodynamic integration using two solvents, polar aprotic (DMSO), and polar protic (water). The kinetic rates were found to be strongly dependent on the solvent polarity; hence, the unbinding rate proceeded much faster in DMSO compared to water. DMSO tends to participate less in a chemical reaction by weakening the intermolecular interaction between chitosan and TouA due to lack of acidic hydrogen resulting in a reduction of the transition state. On the other hand, water, which ought to donate hydrogen atoms, sustains a strong interaction and hence large barrier heights. Consequently, this reduces the unbinding rate and increases the residence time. Binding free energy from thermodynamic integration suggests a thermodynamic stable chitosan-TouA complex in water than in DMSO.

Keywords

Residence time; Solvents; Toussaintine-A; Chitosan; Metadynamics; Kinetics