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Solvent effects on molecular encapsulation of Toussantine-A by chitosan nanoparticle: A metadynamics study

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Solvent effects on molecular encapsulation of Toussantine-A by chitosan nanoparticle: A metadynamics study

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Abstract

We report a metadynamics study of toussantine-A with chitosan nanoparticle in dimethyl sulfoxide and water in order to assess the solvent related effects on free energy and interaction stability between the two compounds. We use well-tempered metadynamics to characterize the binding and unbinding processes of toussantine-A from chitosan. The calculated binding free energies support unbinding process deduced from metadynamics simulation. Toussantine-A interacts poorly with chitosan in the presence of dimethyl sulfoxide when compared to water; the dimethyl sulfoxide gives rising a reverse effect on drug binding that favours to the unbinding of toussantine-A.