

Daniel M Shadrack

Molecular dynamics and related methods in macromolecules-drug interaction

Abstract

Atomistic simulations of materials play an important role in exploring and understanding materials at molecular level. Molecular dynamics simulation, a computation tool, has helped to compliment experimental results and provide atomistic details where experiments have limitation. In this talk, I will discuss the application of molecular dynamics simulation in drugs design, the main focus will be in drug-nanoparticle interaction, protein-ligand interaction and solution conformation of small molecules. Then, I will discuss how molecular dynamics have helped to complement and interpret various experimental results.

Date 19 November 2020