The Role of Molecular Modeling and Related Methods in Drug Design

Daniel M Shadrack

Chemistry Department, St John's University of Tanzania, P.O.Box 47 Dodoma, Tanzania.

Abstract

Over the past two decades, computers simulations, in particular molecular dynamics simulation and its related methods such free energy calculations and enhanced sampling approaches, has accelerated the process of drug discovery. In this talk, the role played by MD simulation in the discovery of antibacterial, anticancer and anti-viral compounds, will be discussed. Some successive examples of drugs discovered by MD simulations will be highlighted. Besides understanding protein-ligand interactions, solvents plays an important role in drug design and are known dictates the biological activity of small molecules (drugs). The heterogeneous interactions at water-small molecule interfaces which drives the self-assembly and aggregation process of hydrophobic drugs in aqueous environment as well as their conformations and orientation preferences will be discussed in detail using niclosamide, capsaicin and linamarin as model molecules. Finally, the self-aggregation process of hydrophobic molecules will be linked with their solubility issues.