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Editorial

Molecular Dynamic Simulations: An Important Aspect in Drug Discovery

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Computational drug discovery today is one the important tools which can accelerate the challenging process of designing and optimizing a new molecule. Molecular dynamic (MD) simulation is one of the important aspects which allow implementation of structure based drug design [1]. Flexibility is crucial feature in predicting the binding of ligand and receptor complex and related thermodynamic and kinetic properties. During molecular recognition process enzymes and receptors undergo conformational change; some with small and some proteins undertake significant conformational changes. Understanding the flexibility of the target receptor through MD simulation will help us to improve the designing of the drugs over the simplistic lock and key conceptualization. These changes in the drug receptor binding involve elements of secondary and tertiary structure and such flexibility of conformational changes is handled by MD simulation [2,3].

Molecular dynamics simulations employ a force field which is used to estimate the forces between interacting atoms and calculate the overall energy of the system. From these MD trajectories varieties of properties can be calculated, including free energy, kinetics measures, and other macroscopic quantities [4]. Experimentally it is not always possible to detain the molecular interactions sequentially and MD simulation helps in understanding these sequential reactions following the biophysical limits. Different boundary conditions such as cylindrical, periodic, spherical are taken care during simulation. Depending on the requirement of the study pressure and temperature are maintained throughout the simulation study [5].

Different theoretical background underlies for the MD simulation which comprises of classical potential, thermodynamic potential and enhanced sampling. The central idea behind MD simulations is to study the time dependent behaviour of microscopic systems and the model derived from the time dependent study refers to the force field and molecular mechanics. Another theoretical approach allows quantitative estimates of important thermodynamic observables to be computed from MD trajectories such as internal energy, heat capacity and pressure. Enhanced sampling method is another theoretical way which was developed to overcome the limitation of Boltzmann sampling [4,6].

Molecular dynamic simulations and its related method could enhance the pace of drug discovery which would offer savings in money and time. It improves the traditional virtual screening methodologies and direct prediction of ligand binding energies, additionally, with the identification of some obscured binding sites. With the help of MD simulations, the future of computer aided drug design is promising with constant improvements in computer power and algorithm design. Thus, MD simulations could play an important role in designing and development of novel pharmacological therapeutics.

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