Computational Chemistry: Application of Molecular Dynamics Simulation and Docking Approaches in Drug Design.

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Abstract

Molecular Dynamics Simulation and molecular docking have become an increasingly important tool for drug research and development. It is now possible to dock libraries of more than ten million molecules against targets over several days on medium sized server. The commercially available molecules may be rapidly tested to find some new leads in a shorter period of time.

In this talk, a brief introduction of the available molecular dynamics simulation, molecular docking methods, and their development and applications in drug discovery are going to be presented. The relevant basic theories, including sampling algorithms and scoring functions, are also discussed. Although the application of docking and scoring has led to some remarkable successes, there are still some major challenges to be solved. A novel and robust automated docking method that predicts the bound conformations of flexible ligands to flexible macromolecular targets is the ultimate goal. In addition, a reasonable scoring function that estimates the free energy change upon binding must be developed. Approaches to address some of these challenges and the latest developments in the area are discussed. A number of successful applications of structure-based molecular modelling and docking results from our studies are going to be presented.