Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Students' Annual Seminar

Study of protein ligand binding using coarse grain simulations

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In recent years the MD simulations have played a very important role in providing the understanding of binding processes in not only in great detail but also with experimental accuracy (simulated bound structure of PL complex matches exactly with the experimental XRD crystal Structure of PL complex). But in spite of advanced developments in the field of MD simulations (such as the use of HPCs and GPUs) we are still limited by the system size which we can handle and the time length scale which we can achieve from unbiased All-atom (AA) MD simulations. Therefore, many interesting and important biological systems are still inaccessible with the AA MD simulation. Here come the advantages of using Coarse Grain (CG) MD simulations over the AA MD simulations. We are using one of the most popular Martini Force Field for Coarse grain simulation.

In the present work, we are going to check the efficiency of Martini FF for studying the binding processes of two protein-ligand systems namely T4lysozyme (L99A) -Benzene binding and CytochromeP450-Camphor binding using CG simulations and compare it with the AA MD simulation results. We are going to ask questions like, at what extent the CG simulations can describe the accurate binding results compare to AA MD simulations? Can they show single as well as multiple paths as seen in the AA MD simulations? Can they provide right kinetics and thermodynamics for protein-ligand binding systems similar to the experimental accuracy? Answers to these questions will allow us implement this CG modelling to other unexplored bigger PL systems and also for longer time length.

Friday, Mar 1st 2019

10:00 AM (Tea/Coffee at 9:45 AM)

Seminar Hall, TIFR-H