TIFR Centre for Interdisciplinary Sciences
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Students' Annual Seminar

Jaya Krishna K

Topic I: Force Field dependence of carbohydrate system

The choice of Force Fields (*ff*) in molecular dynamics simulation plays a crucial role to get accurate results. While protein and lipids have received significant attention on assessing their respective *ff*, the same is not true for carbohydrate. For carbohydrates, the structural study and development of *ff* have been proven difficult because of various issues such as high flexibility of glycosidic linkages and ring conformations, presence of high number of chiral centers, subtle variations in spatial charge distribution, etc. Even though there exists multiple *ff* developed for carbohydrates, they have not been assessed properly for their accuracy till date. In this current work, I have used extensive molecular dynamics simulation of amylose chain to explore the quality of four popular carbohydrate *ff* namely charmm36, GLYCAM06, GROMOS 53a6 and OPLS-AA. The presentation will elaborate on results showing significant conformational heterogeneity across different carbohydrate *ff*.

Topic II: Computer simulation approach to model and study the kinase inhibitor drugs.

Kinase is an enzyme that catalyses phosphorylation process. Any alteration to this kinase activity leads to several diseases. There are many kinase inhibitor drugs in the market to prevent the abnormal kinase activity. But, there is a chance that these kinases may develop resistance to the drugs through mutation.

In my talk I will present my initial results on modeling and parameterization of inhibitor drug's using existing inhibitor drugs as templates.

Thursday, May 25th 2017

4:00 PM (Tea/Coffee at 3:45 PM)

Seminar Hall, TCIS