Institute of Molecular Biology

IMB TechTalk

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"Bioinformatics Methods in Computer Aided Drug Design"

31 January 2012, 11:00 (*s.t.*)

Venue: 2nd Floor Seminar Room
Institute of Molecular Biology (IMB)
Johannes Gutenberg University Campus Mainz

All are welcome to attend

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Abstract:

Bioinformatics Methods in Computer Aided Drug Design

The successful development of new drugs is one of science's most difficult tasks today. Even under optimal circumstances, it takes years to finish, has a very low probability of success, and is immensely expensive. In this talk, I want to highlight how computer science can help to make drug design cheaper, faster, and more reliable. This includes classical Bioinformatics techniques, such as sequencing and network analysis, as well as automated and manual molecular modeling approaches.

In the first part, I will focus on the accurate computation of electrostatic effects which play an important role in the energetics of biomolecules.
Many of those effects are dominated by the shielding effect of the water that is always present in biochemical reactions. Therefore, a highly accurate computation of electrostatic potentials of biomolecules in water is an important precursor for many applications in bioinformatics, like the mentioned computer aided development of inhibitors for disease related enzymes, but also, e.g., for an accurate structural modeling of nucleosomes.

In the second part, I will introduce our recent work in molecular visualization which allows interactive real-time ray tracing of biomolecular systems. The use of such ray tracing techniques can help to greatly improve visual quality and - more importantly - depth and geometry perception by the viewer.