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Rheinische
Friedrich-Wilhelms-
Universität Bonn

Einladung zur Vortragsreihe
Algorithmische Bioinformatik

Herr Prof. Dr. Kay Hamacher, TU Darmstadt

spricht über

Reduced Molecular Models : a Pipeline for in-silico Systemsbiology and Biomolecular Engineering

Datum: Dienstag, 23. Dezember 2008
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Bioinformaticians have developed a multitude of algorithms to understand evolution at the sequence level and annotate evolutionary processes by information theoretical measures, statistical modeling and so forth. In addition ample approaches were suggested to derive systems biological insight by similar means. At the same time Molecular Dynamics simulations became the standard procedure to understand the physical rammifications of such mutations in the molecular phenotype and to investigate particular molecular interactions - alas only a few of them are currently accessible due to large CPU-demands of MD protocols.

In this talk I would like to put forward a third, alternative way to merge the information space (of sequence evolution especially by mutation) with the biophysical reality (the world in which the selective advantage reveals itself) by using reduced molecular models. These models allow at the same time efficient and large-scale investigations into biomolecular networks and the design of functional biomolecules.

To illustrate this I will show recent results on a viral enzyme in HIV, molecular design approaches for ion-channels and how to apply such models to protein-protein-interaction networks occuring in macromolecular self-assembly processes. Implementation & algorithmic issues and future prospects are discussed.