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VABILO NA PREDAVANJE / INVITATION TO THE LECTURE

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Četrtek/ Thursday, 11. 02. 2010, ob / at 13:00

Velika predavalnica Kemijskega inštituta / Lecture Hall at the
National Institute of Chemistry; Hajdrihova 19, Ljubljana

Multiscale Protein Modeling: structure prediction, macromolecular assemblies and folding pathways

Povzetek / Abstract

Protein structure prediction is now feasible for a significant fraction of newly determined sequences. Computationally more challenging is prediction of protein folding pathways. Also theoretical prediction of biomacromolecular assemblies and mechanisms of protein aggregation is still very far from a satisfactory solution.

Since global relaxations of protein structures (including protein folding) is a very slow process, typically lasting microseconds to seconds a straightforward approach via classical methods of molecular mechanics remains impractical, except very small systems. Thus, multiscale approaches based on coarse grained sampling techniques of protein conformational space are frequently applied in structure prediction. Multiscale simulations can also provide insights into protein dynamics and protein-protein interactions.

Obviously, for typical biological applications we need as accurate as possible all-atom models. Therefore, it is necessary to be able to build a reasonable all-atom picture from the reduced structures and trajectories from the lower resolution methods. As it is shown in this contribution, sometimes such multiscale approaches are quite successful.

Vljudno vabljeni! / Kindly invited!

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