BP 20: Posters - Molecular Dynamics

Time: Monday 17:30–19:30 Location: Poster C

BP 20.1 Mon 17:30 Poster C

Competition of Electrostatic vs. Hydrophobic Forces in the Central Core Region of Amyloid beta Fibrils — •Felix Hoffmann, Gül Bekcioglu-Neff, and Daniel Sebastiani — Martin Luther Universität Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle

Amyloidogenic peptides aggregated to large molecular assemblies are a hallmark of several diseases including Parkinson's, Huntington's, and Alzheimer's disease as well as type II diabetes. Despite that each of these diseases gives rise to a very distinctive clinical picture, amyloid fibrils share the cross-beta structure as a common structural feature. Within this structure, peptide strands are linked via lateral beta-sheet-turn-beta-sheet motifs resulting in fibre-like aggregates with diameters of a few nanometers and lengths up to several micrometers.

The central question addressed is how electrostatic and hydrophobic interactions compete within the central core region of Abeta(1-40) fibrils. By means of extensive molecular dynamics simulations we investigated a series of rationally mutated Abeta(1-40) variants which introduce electrostatic forces in the central core region of the fibril. Our study shows considerable structural differences compared to existing models of wild type Abeta(1-40) fibrils. [1] Further, we computed NMR chemical shifts and NMR order parameters which are in good agreement with experimental findings and thus validate our computational approach. [1]

[1] F. Hoffmann, G. Bekcioglu, J. Adler, D. Huster, and D. Sebastiani, in preparation.

BP 20.2 Mon 17:30 Poster C

Molecular Evolution — •Emanuel Gregor Worst[1], Philipp Zimmer[2], Eva Wollrab[1], Karsten Kruse[2], and Albrecht Ott[1] — [1]Saarland University, Biological Experimental Physics, Postfach 151150, 66041 Saarbrücken — [2]Saarland University, Theoretical Biological Physics, Postfach 151150, 66041 Saarbrücken

From the origin of life Darwinian evolution has continuously led to new and different species that make up a highly complex biosphere. Reproduction in conjunction with variation leads to the permanent selection and emergence of new species. How Nature avoids an evolutionary stall and keeps on innovating remains poorly understood. Many aspects of Darwinian evolution have been described by experimental as well as theoretical approaches. However, a realization of Darwinian evolution on long time scales that does not end up in the selection of a single fittest evolutionary winner is still lacking. We introduce an experimental system that consists of linear DNA molecules of a given length that are able to reproduce in a template-directed way. Longer molecules emerge by spontaneous ligation. A DNA species is formed by DNA strands that feed on shorter strands and that eventually outcompete other existing DNA molecules. An evolutionary stall is avoided if these new species serve as a niche that future mutants feed upon. Our molecular evolutionary system is principally able to progress indefinitely.

BP 20.3 Mon 17:30 Poster C

Quantitative assessment of sampling quality of molecular dynamics simulations of biomolecular systems — •Mike Nemec and Daniel Hoffmann — Bioinformatics - Center for Medical Biotechnology, University of Essen, Germany

Typical biomolecular systems have huge, rugged energy landscapes. Although Molecular Dynamics (MD) simulations only sample tiny fractions of these landscapes, these samples are often used for inferring properties of the biomolecular systems, such as thermodynamic averages or conformational states. It is therefore a critical question, how well MD simulations actually sample these systems. Here we show how the quality of the sampling can be assessed by a combination of two measures, the mixture of configurations between MD trajectories and the effective sample size. We report numerical results from extensive MD simulations of two polypeptides in aqueous solution, Met-Enkephalin (5 residues) and HIV-1 gp120 V3 (35 residues), with various sampling protocols, namely conventional MD and two enhanced sampling algorithms aMD and scaledMD.

BP 20.4 Mon 17:30 Poster C

Electrophoretic Mobilization of Neutral Solutes in Salty Solutions — Tomas Krizek[1], Anna Kubickova[1], Pavel Coufal[1], Pavel Jungwirth[2], •Jan Heyda[3], and Vladimir Vladimir[2,3] — [1]Department of Analytical Chemistry, Faculty of Science, Charles University in Prague, Prague, Czech Republic — [2]Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Center for Biomolecules and Complex Molecular Systems, Prague, Czech Republic — [3]Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic

UV-absorbing neutral substances are commonly used as markers of mean electroosmotic flow in capillary electrophoresis. However, it was recently found both experimentally and computationally (dx.doi.org/10.1002/elps.201300544) that some of the markers have dispositions to be mobilized with respect to the electroosmotic flow. The mobilization is caused by interactions of the marker molecule with components of background electrolyte.

In this work, 'amide' markers in combination with selected background electrolyte cations were studied. On the basis of this set of experiments, some general trends in the mobilization of markers were discussed and some favorable and unfavorable marker-cation combinations were pointed out.