SEMINAR

Institute of Molecular Biosciences, University of Graz

27. 11. 2014, 16.00

Seminar room 44.22, Humboldtstr. 48, 2nd floor

On peptide aggregation and novel ways to improve simulations of membrane lipids

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PART I: Computational clarification of structural detail in polyglutamine aggregation

In many neurodegenerative diseases, such as Alzheimer's, Parkinson's and Huntington's, cell death is associated with protein misfolding and aggregation. I discuss the events leading to aggregation of polyglutamine, the aggregation-prone part of the disease- associated protein in Huntington's and eight other diseases. Combining a criterion based on available experimental data with extensive molecular simulations, I demonstrate the infeasibility of many suggested aggregation-initiating structures, and find one motif likely to be crucial for the initiation of aggregation.

PART II: Open online collaboration that uses NMR data to judge the correctness of glycerol backbone and choline head group structures in lipid simulations.

I describe an experiment in open research collaboration that goes by the name NMRlipids. The scientific goal of the project is to test the existing molecular dynamics force fields against published NMR order parameter data. We do this in a fully open way, using a simple blog as the collaboration platform. I describe the one-year-long history (of success) of the project, and on the way will highlight what we have found considering the performance of force fields.