IBPC

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ENS

Understanding the dynamics of protein rare events

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All-atom explicit solvent molecular dynamics (MD) simulations of conformational changes in proteins and protein self-assembly such as folding, binding and aggregation remain a great challenge because of the long time scales involved. These long times are due to high free energy barriers between stable states. While rare event methods, e.g. Umbrella Sampling, Replica Exchange MD, and Metadynamics were developed to overcome these barriers and sample the phase space efficiently, they do not give unbiased kinetics and mechanistic insight. In contrast, Transition Path Sampling (TPS) allows the collection of ensembles of unbiased reactive pathways that can be analysed to do exactly that. In this presentation I will give an overview of the path sampling methodology including recent progress. I will show how one can apply the path sampling methodology in several case studies, including protein conformational changes in signalling proteins, the folding of small proteins, fibril formation, and the role of rotational diffusion in protein binding.

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