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Enhanced Wang Landau Sampling of Adsorbed Protein Conformations MITHUN RADHAKRISHNA, Columbia University, SUMIT SHARMA, Princeton University, SANAT K. KUMAR, Columbia University — Using computer simulations to model the folding of proteins into their native states is computationally expensive due to the extraordinarily low degeneracy of the ground state. In this paper, we develop an efficient way to sample these folded conformations using Wang Landau sampling coupled with the configurational bias method (which uses an unphysical “temperature” which is between the collapse and folding transition of the protein). This method speeds-up the folding process by roughly an order of magnitude over existing algorithms. We apply this method to study the adsorption of HP protein fragments on a hydrophobic surface, a model which is a close analog of one presented recently by Shea and coworkers. We are able to readily capture the fact that these fragments, which are unstructured in the bulk, acquire secondary structure upon adsorption onto a strong hydrophobic surface. Apparently, the presence of a hydrophobic surface allows these random coil fragments to fold by providing hydrophobic contacts that were lost in protein fragmentation.

Prefer Oral Session
 Prefer Poster Session

Mithun Radhakrishna
mr2972@columbia.edu
Columbia University

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