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Structural and Dynamic Analysis on IDPs by Modified AWSEM-MD HAO WU, GAREGIN PAPOIAN, Univ of Maryland-College Park, PAPOIAN THEORETICAL BIOPHYSICS GROUP TEAM — Unlike globular proteins, intrinsically disordered proteins (IDPs) lack both secondary and tertiary structures and can play key roles in various biological processes, including transcriptional regulation, molecular recognition and cellular signaling. These functions can be potentially elucidated by structural heterogeneity of IDPs. Because of their flexibility and disordered nature, it has been difficult to investigate IDPs both computationally and experimentally. In particular, it is desirable to develop coarse-grained, yet accurate models of IDPs, such that simulations exploring sufficient conformational ensembles could be carried out within feasible times. To achieve this goal, we modified the associative memory, water mediated, structure and energy model (AWSEM-MD), which is typically used for folding of globular proteins or binding studies. We tested modified AWSEM-MD on several well-studied IDPs and found the transient secondary structure propensity is consistent with NMR experimental results. The rugged free energy landscapes obtained also show structural heterogeneity of these IDPs. Our proposed extension of AWSEM-MD may allow simulating a wider range of IDPs with high accuracy and computational efficiency.

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