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Predicting folding-unfolding transitions in proteins without a priori knowledge of the folded state[1] OSMAN OKAN, DENIZ TURGUT, ANGEL GARCIA, RAHMI OZISIK, Rensselaer Polytechnic Institute — The common computational method of studying folding transitions in proteins is to compare simulated conformations against the folded structure, but this method obviously requires the folded structure to be known beforehand. In the current study, we show that the use of bond orientational order parameter (BOOP) Q_l [Steinhardt PJ, Nelson DR, Ronchetti M, Phys. Rev. B 1983, 28, 784] is a viable alternative to the commonly adopted root mean squared distance (RMSD) measure in probing conformational transitions. Replica exchange molecular dynamics simulations of the trp-cage protein (with 20 residues) in TIP-3P water were used to compare BOOP against RMSD. The results indicate that the correspondence between BOOP and RMSD time series become stronger with increasing l. We finally show that robust linear models that incorporate different Q_l can be parameterized from a given replica run and can be used to study other replica trajectories.

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