

P003 Caught in Action: Protein-G Oligomerization
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Biochemical processes such as protein folding, binding, and catalysis often occur in microsecond to millisecond. Capturing dynamics motions of proteins in such slow timescale remains a challenging and pertinent goal for investigating the relation of structure, dynamics, and function. We present a multi-scale molecular dynamics approach that allows to sample large conformational changes and to identify important dynamic information. The method is tested on the $\beta 1$ domain (the immunoglobulin-binding domain) of Streptococcal protein-G. Simulation results are analyzed and compared to motions that have been captured as possible mechanisms, explaining how monomer can be induced to form oligomers in previous protein engineering experimental studies. In addition, backbone dynamics order parameters computed from the model-free approach with a double exponential fitting function are highly correlated to those obtained from experimental residual dipole coupling measurements.