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Extracting Protein Dynamics from Single Molecular Time Series

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New experiments using scanning probe microcopies and advanced optical methods allow us to study biological molecules as individuals, not just as populations. The findings of these studies give substantially new information concerning the complexity of biomolecules in a structured environment and lead to new insight into biophysics process on single-molecule level. Based on contemporary single molecule experiments, nonlinear time series and network theory, aiming at developing new theoretical modeling methods, we introduced the concept of “state” and extracted information from single molecular time series. During our research, we used the simulation trajectory data of a 20 residue antiparallel β-sheet peptide from Amedeo Caflisch’s research group to build up a complex network of “state”s. The results are expected to reveal the detailed connections between conformational fluctuations and “state”s, as well as relationship between energy landscape and the complex state network. We will report and discuss the method and the preliminary results.