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Structural Transitions and Aggregation in Amyloidogenic Proteins TIMOTHY STECKMANN, PREM CHAPAGAIN, BERNARD GERSTMAN, Florida Intl Univ, COMPUTATIONAL AND THEOREITCAL BIOPHYSICS GROUP AT FLORIDA INTERNATIONAL UNIVERSITY TEAM — Amyloid fibrils are a common component in many debilitating human neurological diseases such as Alzheimer's and Parkinson's. A detailed molecular-level understanding of the formation process of amyloid fibrils is crucial for developing methods to slow down or prevent these horrific diseases. Alpha-helix to beta-sheet structural transformation is commonly observed in the process of fibril formation. We performed replica-exchange molecular dynamics simulations of structural transformations in an engineered model peptide cc-beta. Several sets of simulations with different number of cc-beta monomers were considered. Conversion of alpha-helix monomers to beta strands and the aggregation of beta strand monomers into sheets were analyzed as a function of the system size. Hydrogen bond analysis was performed and the beta-aggregate structures were characterized by a nematic order parameter.

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