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Structural Transformation and Aggregation of cc-beta Peptides Into Amyloid Proto-fibrils YUBA BHANDARI, TIMOTHY STECKMANN, PREM CHAPAGAIN, BERNARD GERSTMAN, Florida International University, Miami, Florida — The study of amyloid fibrils has important implications in understanding and treatment of various neurodegenerative diseases such as Alzheimer's and Parkinson's. During the formation of amyloid fibrils, peptide polymers manifest fascinating physical behavior by undergoing complicated structural transformations. We examine the behavior of a small engineered peptide called cc-beta, that was designed to mimic the structural changes of the much larger, naturally occurring amyloid beta proteins. Molecular dynamics (MD) simulations are performed to uncover the underlying physics that is responsible for the large scale structural transformations. By using implicit solvent replica exchange MD simulations, we examined the behavior of 12 peptides, initially arranged in four different cc-beta alpha helix trimers. We observed various intermediate stages of aggregation, as well as an organized proto-fibril beta aggregate. We discuss the time evolution and the various interactions involved in the structural transformation.

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