

## **Oligomerization of the (25-35) fragment of the Alzheimer A $\beta$ peptide**

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The A $\beta$ (25-35) peptide is one of the shortest fragments of the Alzheimer amyloid- $\beta$  peptide to possess neurotoxic properties. This peptide is toxic both in its monomeric form, as well as in an oligomeric state. A characterization of the monomeric species of A $\beta$ (25-35) is key to understanding its toxicity and for the identification of conformations that may act as seeds for further growth into fibrils. We present a replica exchange molecular dynamics study of the conformational space accessible to this peptide in explicit solvent. The peptide is seen to adopt a mostly random coil structure, with a smaller population of structured hairpin conformations. Simulations of dimers indicate that aggregation into larger assemblies can be initiated either from the coil state or from the hairpin configurations, resulting in fibrils of different morphologies.