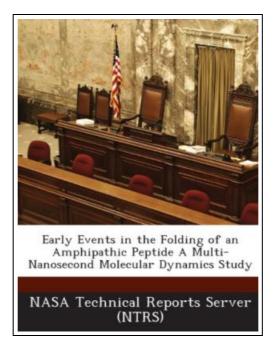
## Early Events in the Folding of an Amphipathic Peptide a Multi-Nanosecond Molecular Dynamics Study (Paperback)



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## Reviews

This composed publication is fantastic. This is certainly for all those who statte that there was not a well worth reading through. You will not truly feel monotony at whenever you want of your respective time (that's what catalogs are for regarding when you ask me). (Prof. Mark Ratke Jr.)

## EARLY EVENTS IN THE FOLDING OF AN AMPHIPATHIC PEPTIDE A MULTI- NANOSECOND MOLECULAR DYNAMICS STUDY (PAPERBACK)



Bibliogov, United States, 2013. Paperback. Condition: New. Language: English . Brand New Book \*\*\*\*\* Print on Demand \*\*\*\*\*. Folding of the capped LQQLLQQLLQL peptide is investigated at the water-hexane interface by molecular dynamics simulations over 161.5 nanoseconds. Initially placed in the aqueous phase as a beta-strand, the peptide rapidly adsorbs to the interface, where it adopts an amphipathic conformation. The marginal presence of non-amphipathic structures throughout the complete trajectory indicate- that the corresponding conformations are strongly disfavored at the interface. It is further suggestive that folding in an interfacial environment proceeds through a pathway of successive amphipathic intermediates. The energetic and entropic penalties involved in the conformational changes along this pathway markedly increase the folding time-scales of LQQLLQQLLQL, explaining why the alpha-helix, the hypothesized lowest free energy structure for a sequence with a hydrophobic periodicity of 3.6, has not been reached yet. The formation of a type I beta-turn at the end of the simulation confirms the importance of such motifs as initiation sites allowing the peptide to coalesce towards a secondary structure.

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