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A thermodynamic study of Abeta(16-21) dissociation from a fibril using computer simulations. CRISTIANO DIAS, FARBOD MAHMOUDINOBAR, ZHAOQIAN SU, New Jersey Institute of Technology — Here, I will discuss recent all-atom molecular dynamics simulations with explicit water in which we studied the thermodynamic properties of Abeta(16-21) dissociation from an amyloid fibril. Changes in thermodynamics quantities, e.g., entropy, enthalpy, and volume, are computed from the temperature dependence of the free-energy computed using the umbrella sampling method. We find similarities and differences between the thermodynamics of peptide dissociation and protein unfolding. Similarly to protein unfolding, Abeta(16-21) dissociation is characterized by an unfavorable change in enthalpy, a favorable change in the entropic energy, and an increase in the heat capacity. A main difference is that peptide dissociation is characterized by a weak enthalpy-entropy compensation. We characterize dock and lock states of the peptide based on the solvent accessible surface area. The Lennard-Jones energy of the system is observed to increase continuously in lock and dock states as the peptide dissociates. The electrostatic energy increases in the lock state and it decreases in the dock state as the peptide dissociates. These results will be discussed as well as their implication for fibril growth.

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