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Oligomerization of the protein tau in the Alzheimer's disease LUCA LARINI, Rutgers University - Camden — The Alzheimer's disease is characterized by the formation of protein aggregates both within and outside of the brain's cells, the neurons. Within the neurons, the aggregation of the microtubule associated protein tau leads to the destruction of the microtubules in the axon of the neuron. Tau is extremely flexible and is classified as an intrinsically disordered protein due to its low propensity to form secondary structure. Tau promotes tubulin assembly into microtubules, which are an essential component of the cytoskeleton of the axon. The microtubule binding region of tau consists of 4 pseudo-repeats that are critical for aggregation as well. In this study, we focus on the aggregation propensity of different segments of the microtubule binding region as well as post-translational modifications that can alter tau dynamics and structure. We have performed replica exchange molecular dynamics simulations to characterize the ensemble of conformations of the monomer and small oligomers as well as how these structures are stabilized or destabilized by mutations and post-translational modifications.

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