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Computational Study of Pseudo-Phosphorylation and Phosphorylation of the Microtubule Associated Protein Tau DMITRIY PROKOPOVICH, student, LUCA LARINI, Professor — This study focuses on the effect of pseudo-phosphorylation on the aggregation of protein tau, which is very often found interacting with microtubules in the neuron. Within the axon of the neuron, tau governs the assembly of microtubules that make up the cytoskeleton. This is important for stabilization of and transport across the microtubules. One of the indications of the Alzheimer's disease is the hyper-phosphorylation and aggregation of protein tau into neurofibrillary tangles that destroy the neurons. But even experts in the field do not know if hyper-phosphorylation directly causes the aggregation of tau. In some experiments, pseudo-phosphorylation mimics the effects of phosphorylation. It does so by mutating certain residues of the protein chain into charged residues. In this computational study, we will employ a fragment of tau called PHF43. This fragment belongs to the microtubule binding region and papers published by others have indicated that it readily aggregates. Replica exchange molecular dynamics simulations were performed on the pseudo-phosphorylated, phosphorylated, and dimerized PHF43. The program used to simulate and analyze PHF43 was AMBER14.

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