

Molecular Dynamics of the Cargo Binding Domain of the Kinesin-1 Motor Protein

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Alzheimer's is the leading cause of dementia in the elderly. The little information that is known about the disease comes from the rarest form of Alzheimer's known as Familial Alzheimer's Disease, which accounts for less than 5% of those afflicted. It is believed that Familial Alzheimer's disease is caused by mutations in three different gene products; Presenilin 1 (PS1), Presenilin 2 (PS2), and Amyloid Precursor Protein. This study sought to understand the dynamics of the cargo binding domain of the Kinesin Light Chain-1; the motor protein hypothesized to transport the Amyloid Precursor Protein (APP). To understand the dynamics of the Kinesin Light Chain-1 (3NF1) and the extended conformation of the C-terminal of APP, long time scale molecular dynamics simulations were performed on both structures using DESMOND and force fields: Amber99SB, Charmm22*, and Charmm27. The results indicate the dynamics of 3NF1 and suggest a possible structure for the C-terminal tail of the Amyloid Precursor Protein.