

# **Investigating the Apo-Dynamics of JIP-1**

Lauren McRae, Erica Modeste, Cooper Taylor, Carol Parish  
University of Richmond

The Parish research group is working on the hypothesis that Kinesin Light Chain protein (KLC) is responsible for transporting amyloid precursor protein (APP), and misregulation of this process is a causative factor in Alzheimer's disease. Recent experiments indicate that C-Jun Amino-Terminal Kinase-Interacting Protein-1 (JIP-1) is likely important in the binding of KLC and APP. Very little is known about JIP-1, and because it could be a vital component of APP transport, molecular dynamics (MD) simulations using AMBER 14 were used to study the apo-dynamics of this protein. It has been indicated experimentally that 11 residues within the JIP-1 protein retain the function of the molecule as a whole, so an extended 70 residue strip including the aforementioned residues was studied in these simulations. 100ns of conventional MD was performed on JIP-1 in three different simulations, followed by constant pH MD and pH Replica Exchange MD to observe the pH dependence of the molecule. Understanding these properties could explain much about the conformation and folding of this protein.