

Structural Point Mutations of p53 Protein and Their Effects on the Zinc Coordination Complex

Taylor Quinn, Kelly M. Thayer
Department of Chemistry, Vassar College
Poughkeepsie, NY

The p53 protein is an important transcription factor in the cell cycle. As such, mutations of this protein are found in at least 50% of all cancers, most of which are in the “core-domain” containing residues 102-292. This research is focusing on the molecular dynamics of p53 with point mutations that affect the structural stability of the protein, namely, R175H, R282W, G245S, and R249S. The system will be evaluated in reference to the Zn^{2+} tetrahedral coordination complex and its changes, as it has been shown to have an important structural role in relation to the L2 and L3 loops. Previous research has shown that there are five different clusters of DNA sequences that the protein binds to, and all are being evaluated in reference to the p53 protein and its mutations. The molecular dynamics are being run and evaluated using AMBER, tleap, and VMD. Results and analysis will be presented.