Molecular Simulation on the Compatibility of PTEN and Glioma tumor suppressor candidate region gene 2 protein

PTEN, a type of tumor suppressor protein, is one of the most commonly known carcinogenic genes when mutated. It has been identified that in tumors found in glioblastomas, endometrial, and prostate cancers, somatic deletions and mutations in the PTEN gene were prominent (Cristofano and Pandolfi, 2000). This phenomenon causes a disruption in the AKT/ PI3K pathway in which PTEN ceases to hydrolyze PIP3 preventing the conversion from PIP2 to PIP3 (Wang, 2010). The disruption of these pathways induces cell growth, cell cycle progression, and inhibits apoptosis thus making the PTEN gene a proto-oncogene. Systematic errors caused by PTEN are due to the protein misfolding and reannealing to itself resulting the protein to be inactive. That is why it is essential to understand the nature of PTEN and how PTEN interacts with other proteins. In this experiment, a simulation will be done in Visual Molecular Dynamics and NAMD to see the behavior of the binding energies with a known protein, Glioma tumor suppressor candidate region gene 2 protein, which will be termed 40-1. A more detailed analysis will be conducted to further see where PTEN and 40-1 are most intermolecularly compatible and the total binding energies that are associated with these regions.