Introducing Hierarchical Aspect to Protein Residue Principle Component Analysis for Molecular Dynamics Simulation of Recombinant Vaccine to Detect Vital Alpha Carbon Motions

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The focus of this research is to computationally elucidate the motion in a recombinant vaccine to detect vital alpha carbon motions. To correct for PCA's insufficiencies, a hierarchical analysis will be introduced to the analysis in which residue alpha carbon motion is correlated and co-varied with larger-scale subsection motions. The focus of this study will be to quantify the component analysis of the proteins in this dataset based on hierarchical aspects, and to perform comparisons between the various proteins. This work will represent an extension to previous results that characterize the mechanisms underlying thermodynamic stability and intrinsic flexibility. Normal PCA processes all information in one calculation and risks missing fine motions that can be important to function, which the hierarchical analysis corrects for through subsection motion correlation and covariance analysis. Through applying the hierarchical perspective, insight into the shortcomings of standard PCA can be gained allowing for heightened computational analyses through the utilization of this method. These results underscore the reason for why difficulties are encountered in protein design and alpha carbon motion analysis. Necessities for the experimental methods of this project will include the use of a computer with a Unix based operating system, MD simulation software package, a specialized program called Java Essential Dynamics that performs principal component analysis (PCA) on all-atom trajectories, graphing software, molecular visualization software called VMD, mathematics software called MATLAB, in which the hierarchical aspect is introduced to the analysis. Experimentation will consist of vaccine (RiVax) and its mutant, both analyzed through the standard and hierarchical analysis.

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