



**CALIFORNIA STATE SCIENCE FAIR
2013 PROJECT SUMMARY**

Name(s) Raghu V. Dhara	Project Number S1506
Project Title A Novel Pentameric Model of the T4 Bacteriophage Genome Packaging Motor and a Means of Disrupting Its Mechanism	
<p style="text-align: center;">Abstract</p> <p>Objectives/Goals The first objective of this project is to determine the exact structure of the protein complex that comprises the T4 bacteriophage's molecular motor. The second objective is to provide a mechanism by which the model proposed in step one would package the DNA. The final objective is to discover a molecule that would effectively disrupt motor function and disable the virus. This project has immense potential in medicine, as the drug molecule proposed in phase three can be refined to produce more effective antiviral drugs.</p> <p>Methods/Materials Phase one was accomplished using rotation matrices, Java code, molecular visualizers such as VMD, and a previously proposed conformation as a starting point; with these tools, a stable, feasible structure that met all criteria, both theoretical and experimental, was designed. Phase two used biomolecular computer simulation software like NAMD and Chimera. The molecular cap from phase three was found using molecular docking software, namely AutoDock Vina.</p> <p>Results Based on the analysis of data from molecular visualizers, I propose a novel configuration for the T4's motor. It resembles a cone without its apex, commonly known as a frustum. Using this frustum shape, molecular modeling, and mathematical analysis, I offer a new model for the translocation of genetic material through the virus, known as the "frustum-impulse" model after the motor's shape and primary physical principle of operation. Finally, human phospholamban protein, or PLN, looks to be a feasible molecular cap that completely inhibits motor operation.</p> <p>Conclusions/Discussion We have concluded that the shape of the viral packaging motor is a frustum, that the model for translocation is the frustum-impulse mechanism, and that PLN can effectively disrupt the T4 motor function. Still, much work needs to be done: frustum impulse must be tested experimentally and the phospholamban cap should be examined more closely to determine its drug potential. In any event, this project has advanced our understanding of nature's most mysterious pathogens and offered a possible means of addressing numerous illnesses that plague our society.</p>	
Summary Statement This project attempts to obtain the structure of a viral genome packaging motor, offers a model for how the motor functions, and provides a possible way to disrupt its mechanism.	
Help Received Worked with UCSD NanoEngineering Department with Professor Gaurav Arya	