REBECCA RUTHERFORD and ERICA HARVEY, Dept. of Natural Sciences, Fairmont State University, Fairmont, WV 26554, and BLAKE MERTZ, Dept. of Chemistry, West Virginia University, Morgantown, WV 26506. Molecular dynamics investigation of surfactant micelles as a potential drug delivery vehicle.

A new molecular dynamics study is being initiated in which micellar structures of cetyltrimethylammonium bromide (CTAB) are simulated within computationally constructed physiological conditions. Leading up to the simulation phase, several programs and reference files were used to construct a topology file, initial structure/coordinate files, and parameter files to accurately represent a single molecule of CTAB. This single molecule is utilized in making the initial configuration of a system. All systems begin in one of three configurations: a random assembly of molecules in a box, a pre-formed micelle, or an inverse micelle. These initial configurations, once assembled, are placed under generated physiological conditions by using Visual Molecular Dynamics (VMD) to solvate the system with water and add Na+ and Cl- ions to neutralize the system to 0.15 M NaCl, then using Nanoscale Molecular Dynamics (NAMD) to minimize energy and heat the system to 310 K. The system is then simulated using NAMD until a micelle has formed and stabilized. Following each simulation, quantitative and qualitative analysis is used to characterize the system. The overarching goal of this study is to determine the viability of CTAB as a drug carrier in a targeted drug delivery system. Funding for the project is provided by the College of Science and Technology at Fairmont State University and the NASA WV Space Grant Consortium.