ASHLEY HOFFMASTER#, BRITTANY BONNETT, SADEGH FARAMARZI, DANIELLE GRODI, BLAKE MERTZ, and ERICA HARVEY, Department of Biology, Chemistry and Geoscience, Fairmont State University, Fairmont, WV, 26554**. Molecular dynamics investigation of dodecylmaltoside micelle properties.**

Micelles are spherical assemblies of detergent molecules that form in aqueous solutions. The hydrophilic head of each molecule faces water on the outside of the sphere and the hydrophobic tail of the molecule points toward the center of the micelle. While detergent micelles are commonly used to mimic cell membranes during experimental work on membrane proteins, their biophysical properties are not well understood at the atomistic level. The present work focuses on all atom molecular dynamics simulations of the detergent molecule dodecylmaltoside (DDM). We have investigated the effects of starting configurations and total number of molecules in the simulation (above and below the aggregation number) using pre-formed micelle arrangements consisting of 60, 80, 100, 130, 150, and 200 DDM molecules and random assortment arrangements of 60, 110, 200, and 220 DDM molecules. Results to be presented include validation of the CHARMM force field for DDM, aggregation number, and radius of gyration.